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Monte Carlo Sampling-Based Methods in Stochastic Programming

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Dedicated to the loving memory of my father, Erdoğan Bayraksan, who taught me so much. Also dedicated to my mother, Dr. Gülsen Bayraksan and my brother, Ömer Bayraksan, for their love and support.

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Monte Carlo Sampling-Based Methods in Stochastic Programming

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Many problems in business, engineering and science involve uncertainties but optimization of such complex systems is often done in practice with deterministic model parameters. Stochastic programming extends deterministic optimization by incorporating random variables and probabilistic statements. A major challenge in the analysis of large-scale stochastic systems is having to consider a large number, sometimes an infinite number, of scenarios. This usually leads to intractable models, even when specially-designed algorithms are used. A natural question that arises then is how to use a limited number of these scenarios and still obtain reasonable solutions to our problems. In this dissertation, we focus on Monte Carlo sampling-based methods for solving large-scale stochastic programs.

Given a candidate solution, suggested as an approximate solution to the original problem, the first question we address is how to assess its quality.

Determining whether a solution is of high quality (optimal or near optimal) is a fundamental question in optimization theory and algorithms. We define quality via the optimality gap and develop sampling-based procedures to form confidence intervals on this gap. Compared to an earlier procedure that requires solution of many optimization problems, our procedures require solving only one or two optimization problems. We discuss a number of enhancements to our basic procedure and present computational results.

Next, we develop sequential sampling procedures for assessing solution quality, which control the sampling error of the confidence interval on the optimality gap. We present two methods, a fully sequential method, where we increase the sample size one by one, and an accelerated method, where we increase the sample size in jumps. We prove asymptotic validity of these confidence intervals and present computational results.

Finally, using our results on assessing solution quality, we propose a sequential sampling procedure to solve stochastic programs. In this procedure, the sample size is sequentially increased until a stopping criterion is satisfied. The stopping rule depends on the optimality gap estimate of the current candidate solution and its sampling variance. We show asymptotically that this procedure finds a solution within a desired quality tolerance with high probability. We present preliminary computational results and discuss implementation issues.

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Chapter 1

Introduction

In this dissertation, we consider a stochastic optimization problem of the form

$$z^* = \min_{x \in X} E f(x, \tilde{\xi}), \tag{SP}$$

where f is a real-valued function that determines the cost of operating with decision x under a realization of the random vector $\tilde{\xi}$, whose distribution is assumed known. $X \subseteq \mathbb{R}^n$ denotes the set of constraints that the decision vector x must obey and E is the expectation operator. The objective in (SP) could be to minimize the expected cost or maximize utility. Or, when f is taken as an indicator function of an event, then the above model minimizes the probability of that event. As simple as it is to state, (SP) represents a large class of problems that can be found in the statistics and operations research literature. For instance, classical maximum likelihood estimation can be cast as above where $-f$ is the log-likelihood function. Many problems in simulation can also be stated as (SP). For instance, one might be interested in minimizing the average work-in-process in a queueing network by allocating buffer capacity or servers.

We mainly focus on a special class of (SP), known as *stochastic pro-*

grams with recourse. The well-known two-stage stochastic linear program with recourse was introduced independently by [7, 15], in which

$$f(x,\tilde{\xi}) = cx \; + \; \min_{y \geq 0} \; \tilde{q}y$$
$$\text{s.t} \quad \tilde{W}y = \tilde{r} - \tilde{T}x,$$

$X = \{x : Ax = b, x \geq 0\}$ and $\tilde{\xi} = (\tilde{q}, \tilde{W}, \tilde{r}, \tilde{T})$ is a random vector on $(\Xi, \mathcal{B}, P)$. This formulation can be extended to multiple stages, integer restrictions can be imposed in any of the stages and nonlinear constraints and objective function terms can be added. Stochastic programs with recourse have been successfully applied to a wide range of problems arising in finance, energy, telecommunications, transportation, logistics and supply-chain management (e.g., [66]). Below we give two examples of stochastic programs with recourse. The first one is a production planning and the second one is a multi-stage financial planning problem. We use the first problem in our computational results in Chapter 2.

Example 1.1 (Capacity Expansion Planning in Manufacturing). *Consider production of m types of products on n flexible machines. Any type of product can be produced on any of the machines but with different costs. Installing capacity on the machines is costly and has to be done before the random demand for the different products is known. Weekly production plans, i.e., assignment of numbers of products of each type to be produced on each machine, can be done after the demand is realized. There is also the option of subcontracting production of some parts, at a higher cost. The aim is to find how*

much flexible capacity to add to each of the machines so that the capacity expansion costs and the expected weekly production costs are minimized. For a mathematical formulation of this problem see [29].

Example 1.2 (Multi-stage Financial Planning). *We have an initial wealth of W_0 and can invest in stocks and bonds. There are $t = 1, \ldots, T$ time periods to invest and at the end of each period, we can rebalance our portfolio. The returns on stocks and bonds are random. The aim is to find an investment strategy so that the expected utility of the wealth at the end of period T is maximized. Formulation of a more general version of the problem can be found in [56].*

1.1 Motivation

In many problems of practical size, the dimension of the random vector $\tilde{\xi}$ is quite large, making (SP) harder to solve. For continuous random vectors, minimization aside, taking the expectation that appears in the objective function might be very difficult when the dimension of the integral is high. For discrete random vectors, the problem size can grow exponentially in this dimension. Therefore, unless the cost function f has a simple structure, or the number of realizations is small, it is often impossible to solve (SP) exactly. In such cases, an intuitive approach is to resort to sampling and approximate the problem with

$$z_n^* = \min_{x \in X} \frac{1}{n} \sum_{i=1}^{n} f(x, \tilde{\xi}^i). \qquad (\mathrm{SP}_n)$$

The observations $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^n$ may be independent and identically distributed (i.i.d.) as $\tilde{\xi}$ or may be generated according to another sampling scheme. Let x^* denote an optimal solution to (SP) with optimal value z^*. Similarly, let x_n^* and z_n^* denote an optimal solution and the optimal cost of (SP$_n$). Consistency and other asymptotic properties of estimators x_n^* and z_n^* have been studied extensively in the literature, see e.g., [3, 19, 38, 59]. For instance, it is well known that under relatively mild conditions, $z_n^* \to z^*$ and all limit points of $\{x_n^*\}$ solve (SP) with probability one (w.p.1) as n grows large. We state the latter result in this form because (SP) may have multiple optimum solutions. Of course, if x^* is unique, the result is that $x_n^* \to x^*$, w.p.1.

The main motivation for the research presented here lies in the question, "What should the sample size n be to have a *good* approximating solution?" More specifically, we ask the question, "Can we come up with a procedure to sequentially increase the sample size and stop at a sample size when a desired precision is reached?" That is, we start with an initial sample size, say n_0, and find $x_{n_o}^*$and $z_{n_o}^*$. If this is a provably good solution, we stop. If not, we increase the sample size to $n_1 > n_0$ and compute $x_{n_1}^*$ and $z_{n_1}^*$. We continue until we reach a good solution. Several issues arise with respect to the sequential sampling procedure described above. For instance,

- How do we know the solution at hand is a good solution? How do we define *good*?
- How do we define rules to increase the sample sizes?
- When do we stop?

- When we stop, can we make statements regarding the quality of the solution obtained?

This dissertation aims to answer questions such as the ones above. For instance, to this end, we define the quality of a solution as its optimality gap and we present procedures that form confidence intervals on the optimality gap of a given candidate solution. We then present a sequential sampling procedure such as the one described above, in which the candidate solution is not fixed but is rather a sequence of feasible solutions that could come from solving a sequence of approximating problems or from another approach.

1.2 Assumptions and Definitions

As we have mentioned earlier, (SP) represents a large class of problems, and the research presented in this dissertation is triggered by a special class of (SP) known as stochastic programs with recourse. That said, we do not restrict ourselves to this class and we consider stochastic programs that satisfy the assumptions stated in this section. We assume the distribution of $\tilde{\xi}$ is known and that we can sample from it. We also assume that the distribution of $\tilde{\xi}$ does not depend on the decision x. We make the following assumptions with respect to (SP):

(A1) $f(\cdot, \tilde{\xi})$ is continuous on X, w.p.1,

(A2) $E \sup_{x \in X} f^2(x, \tilde{\xi}) < \infty$,

(A3) $X \neq \emptyset$ and is compact.

For stochastic programs with recourse, the first assumption is satisfied, for instance, by a two-stage stochastic linear program provided it has relatively complete recourse (i.e., for each feasible first stage decision, it is possible to find a feasible second stage decision, w.p.1). However, it eliminates consideration of two-stage stochastic integer programs when there are integrality constraints in the second stage. The second assumption guarantees existence of second moments and provides a needed uniform integrability condition. In some instances of (SP), X may naturally appear as an unbounded set. However, in most practical problems, a decision-maker would not be averse to specifying possibly large, but finite, simple bounds, $l \leq x \leq u$, making the feasible region bounded and hence compact, if also closed.

In the remainder of this section, we review some statistical terms that we use throughout the dissertation. Suppose we are trying to estimate an unknown scalar parameter, μ. Given a set of random data, the two most common ways to address this question are, either to find a "best estimate" for μ or, to give a range of values in which μ could lie. The former is called a *point estimate* and the latter is an *interval estimate*. Similarly, a *point estimator* is a rule that gives a point estimate and an *interval estimator* is a rule that gives an interval estimate using a set of random data. We denote the point estimator that uses a sample size of n as $\tilde{P}_n$, and an interval estimator as $\tilde{I}_n$. There are many ways to define the quality of an estimator. One of the important desired properties of a point estimator is *consistency*. That is, as the sample size grows, we would like the estimator to converge to the parameter of interest.

We give a formal definition below.

Definition 1.1. $\tilde{P}_n$ is a *consistent estimator* of parameter μ, if for every $\epsilon > 0$, $\lim_{n\to\infty} P(|\tilde{P}_n - \mu| < \epsilon) = 1$.

Note that this definition of consistency requires convergence in probability. For interval estimators, two of the most important factors that determine their quality are *size* and *coverage probability*. Size is the range of values in which μ is inferred to lie and coverage probability is the probability that μ lies within this range. Ideally, an interval estimator is desired to have the smallest possible size with the greatest possible coverage probability. However, the two conflict, as one can always increase the coverage probability by increasing the size. We formally define coverage probability below.

Definition 1.2. *Coverage probability* of an interval estimator is the probability that the random interval $\tilde{I}_n$ contains the parameter of interest, i.e., $P(\mu \in \tilde{I}_n)$.

We sometimes refer to the coverage probability simply as the *coverage*. Interval estimators are usually referred to as *confidence intervals*, and are typically accompanied by a measure of confidence which is an (asymptotic) coverage probability or a lower bound on the coverage probability. If the confidence interval (CI) (asymptotically) has the desired coverage probability then, it is an *(asymptotically) valid* CI. For instance, a $(1-\alpha)$-level confidence interval is asymptotically valid if $\lim_{n\to\infty} P(\mu \in \tilde{I}_n) \geq 1 - \alpha$. In this dissertation, we develop procedures that give confidence intervals on the optimality gap of a candidate solution, or a sequence of candidate solutions. We prove

asymptotic properties concerning the coverage probabilities of our procedures' confidence intervals as the sample size grows large, and we empirically assess these coverage probabilities using small or moderate sample sizes.

A Note on Reporting Coverage Results:

In our computational results, we report coverage probabilities. Suppose we are forming a confidence interval $\tilde{I}_n$ using a sample size of n. We repeat this procedure k times using independent streams of observations. Let us denote the k different interval estimates as $\tilde{I}_n^1, \tilde{I}_n^2, \ldots, \tilde{I}_n^k$. We estimate the coverage probability $P(\mu \in \tilde{I}_n)$ by the number of times $\tilde{I}_n^i$, $i = 1, \ldots, k$ contains μ divided by k. Let's call this quantity $\hat{p}_n$. Note that $\hat{p}_n$ is a (scaled) binomial random variable with parameters $P(\mu \in \tilde{I}_n)$ and k. Therefore, for sufficiently large values of k, we can use the central limit theorem to form a confidence interval on the actual coverage probability, $P(\mu \in \tilde{I}_n)$. For instance, a 90% confidence interval is computed as $\hat{p}_n \pm 1.645(\hat{p}_n(1-\hat{p}_n)/k)^{1/2}$. We report this interval in the computational results presented throughout the dissertation. Note that this is a standard way to report coverage results in the simulation literature, e.g., [41, pp. 508-509].

1.3 Outline of the Dissertation

We begin each chapter with an introduction and a review of relevant literature. We then present the main contributions. We test our procedures using problems from the literature and discuss issues that arise in implementation. We end each chapter with concluding remarks. The rest of the dissertation is

outlined below.

In Chapter 2, we develop Monte Carlo sampling-based procedures for assessing solution quality in stochastic programs. Quality is defined via the optimality gap and our procedures' output is a confidence interval on this gap. The fixed candidate solution is input to the procedures. Compared to an earlier method that requires solution of, say, 30 optimization problems, we present a result that justifies solving only one optimization problem. We call this the single replication procedure (SRP). Even though SRP is computationally significantly less demanding, the resulting confidence interval might have low coverage probability for some problems when a small sample size is used. We provide variants of this procedure that require solution of two optimization problems instead of one and that perform better empirically. We present computational results, discuss when the procedures perform well and when they fail and propose methods to further enhance the performance of the procedures.

In Chapter 3, we develop sequential sampling methods for assessing solution quality of stochastic programs. As in Chapter 2, we fix the candidate solution and develop sequential sampling procedures to control the sampling error. We first present a method, which we call fully sequential procedure, where we increase the sample size one by one. Then, we develop an accelerated method where the sample size is increased in jumps. We stop when the sampling error falls below a desired width. Unlike the methods presented in Chapter 2, the sample size when the procedure stops is now a random variable.

As a result, proving asymptotic validity of the procedures' confidence intervals requires a somewhat different type of analysis.

In Chapter 4, we present a sequential sampling procedure to solve stochastic programs. Given a sequence of candidate solutions with limit points that solve (SP), we assess their quality using methods developed in Chapter 2. As in Chapter 3, the stopping time is random, and here it depends on the relative values of the optimality gap estimate and its sample variance estimate. The sequence of candidate solutions can be found by solving a series of sampling problems with increasing sample size, or, they can be found in another way. We show that this procedure stops in a finite number of steps with probability one and finds a solution within a confidence region with a desired probability, that is again asymptotically valid. We discuss implementation issues and present computational results.

We conclude the dissertation with Chapter 5, where we provide a summary of contributions and discuss future research directions. The material presented in Chapter 2 can be found in [6], and an earlier version of Chapter 2's single replication result has been published in [5].

Chapter 2

Assessing Solution Quality: Fixed-Sample Size Procedures

In this chapter, we develop Monte Carlo sampling-based procedures for assessing solution quality in stochastic programs. Determining whether a solution is of high quality (optimal or near optimal) is a fundamental question in optimization theory and algorithms. For instance, the well-known simplex method for linear programming terminates with an optimal solution when the reduced costs are all nonnegative. The Karush-Kuhn-Tucker conditions provide necessary and sufficient conditions for optimality for certain classes of problems.

Given a candidate solution $\hat{x}$, we define its quality by its optimality gap,

$$\mu_{\hat{x}} = Ef(\hat{x}, \tilde{\xi}) - z^*.$$

There are two difficulties associated with computing this quantity. First, z^* is not known and a lower bound (since we have a minimization problem) on z^* needs to be computed. In integer programming and nonlinear programming, for example, lower bounds are also useful for proving solution quality and are typically obtained through relaxed problems, where either the integrality

constraints or some other complicating constraints are relaxed. An upper bound on z^* is readily available as the cost of the candidate solution. For stochastic programs, a second difficulty is that for a given $\hat{x} \in X$, it is not always possible to compute $Ef(\hat{x}, \tilde{\xi})$ exactly.

Monte Carlo simulation-based methods allow us to estimate an upper bound on the optimality gap for stochastic programs. In the next section, we briefly review how to construct confidence intervals (CIs) on the optimality gap using a multiple replications procedure [43]. Then, we show how to obtain a valid CI using only a single replication. In Section 2.3, we provide variants of this procedure that use two replications. In Section 2.4, we compare the empirical coverage results of the procedures for a newsvendor problem and for two-stage stochastic linear programs with recourse. In Section 2.5, we give more insight on the procedures' performance and we propose using ε-optimal solutions to strengthen that performance. Finally, Section 2.6 contains concluding remarks and a summary.

2.1 Review of Multiple Replications Procedure

In this section, we first review a multiple replications procedure to form CIs on the optimality gap [43]. We then briefly list other work on assessing solution quality of stochastic programs that also use Monte Carlo sampling-based methods.

Let $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^n$ be i.i.d. from the distribution of $\tilde{\xi}$. Then, by interchanging minimization and expectation we obtain a statistical lower bound on

z^*,

$$Ez_n^* = E\left[\min_{x\in X}\frac{1}{n}\sum_{i=1}^{n} f(x,\tilde{\xi}^i)\right] \leq \min_{x\in X} E\left[\frac{1}{n}\sum_{i=1}^{n} f(x,\tilde{\xi}^i)\right] = \min_{x\in X} Ef(x,\tilde{\xi}) = z^*. \tag{2.1}$$

This result establishes that z_n^* has a negative bias, $Ez_n^* - z^* \leq 0$. It can also be shown that $Ez_n^* \leq Ez_{n+1}^*$ for all n. This monotonicity result tells us that on average we obtain better estimates of the optimal value as the sample size increases.

Given a feasible decision $\hat{x} \in X$ and a sample size n for (SP_n), we bound the optimal value of (SP) using the above lower bound result, $Ez_n^* \leq z^* \leq Ef(\hat{x},\tilde{\xi})$. The right inequality comes from suboptimality of $\hat{x}$. An upper bound on the optimality gap for $\hat{x}$ is then $Ef(\hat{x},\tilde{\xi}) - Ez_n^*$. We estimate this quantity by

$$G_n(\hat{x}) = \frac{1}{n}\sum_{i=1}^{n} f(\hat{x},\tilde{\xi}^i) - \min_{x\in X}\frac{1}{n}\sum_{i=1}^{n} f(x,\tilde{\xi}^i). \tag{2.2}$$

The first term on the right-hand side of (2.2) is an upper bound estimate and converges to $Ef(\hat{x},\tilde{\xi})$, w.p.1, by the strong law of large numbers. The second quantity, z_n^*, is a lower bound estimate on z^*. In expectation, it provides a lower bound and under (A1)-(A3) from Chapter 1, Section 1.2 converges to z^*, w.p.1 (see subsequent Proposition 2.1). When a common stream of random numbers, $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^n$, is used in calculating both terms in (2.2), $G_n(\hat{x}) \geq 0$, w.p.1. This approach also facilitates variance reduction.

Because of the minimization in (2.2), $G_n(\hat{x})$ (or, its scaled version $\sqrt{n}(G_n(\hat{x}) - \mu_{\hat{x}})$) is, in general, not normally distributed even as n grows

large. Therefore, in [43] confidence intervals are constructed by employing batch means, an approach frequently used in simulation for estimating the mean of a random variable with an unknown or non-normal distribution. We summarize below the multiple replications procedure (MRP) to construct a CI on the optimality gap. Let $t_{n,\alpha}$ be the $1-\alpha$ quantile of the Student's t distribution with n degrees of freedom.

MRP:

Input: Desired value of $0 < \alpha < 1$ (e.g., $\alpha = 0.10$), sample size n, replication size n_g and a candidate solution $\hat{x} \in X$.

Output: $(1-\alpha)$-level confidence interval on $\mu_{\hat{x}}$.

1. For $i = 1, 2, \ldots, n_g$,

    1.1. Sample i.i.d. observations $\tilde{\xi}^{i1}, \ldots, \tilde{\xi}^{in}$ from the distribution of $\tilde{\xi}$,

    1.2. Solve (SP_n^i) using $\tilde{\xi}^{i1}, \ldots, \tilde{\xi}^{in}$ to obtain x_n^{i*},

    1.3. Calculate $G_n^i(\hat{x}) = \frac{1}{n}\sum_{j=1}^{n}\left(f(\hat{x}, \tilde{\xi}^{ij}) - f(x_n^{i*}, \tilde{\xi}^{ij})\right)$.

2. Calculate gap estimate and sample variance by

$$\bar{G}(n_g) = \frac{1}{n_g}\sum_{i=1}^{n_g} G_n^i(\hat{x}) \quad \text{and} \quad s_G^2(n_g) = \frac{1}{n_g - 1}\sum_{i=1}^{n_g}\left(G_n^i(\hat{x}) - \bar{G}(n_g)\right)^2.$$

3. Output one-sided CI on $\mu_{\hat{x}}$,

$$\left[0, \bar{G}(n_g) + \frac{t_{n_g-1,\alpha} s_G(n_g)}{\sqrt{n_g}}\right]. \tag{2.3}$$

Even though $G_n(\hat{x})$ may not be normal, since $\bar{G}(n_g)$ is a sample mean of i.i.d. random variables, it is possible to use the standard central limit theorem

(CLT) to construct an approximate $(1-\alpha)$-level CI for the optimality gap given in (2.3). Due to the negative bias of z_n^*, $E\bar{G}(n_g) \geq Ef(\hat{x},\tilde{\xi}) - z^*$. Thus, for sufficiently large n_g, we can infer that

$$P\left(Ef(\hat{x},\tilde{\xi}) - z^* \leq \bar{G}(n_g) + \frac{t_{n_g-1,\alpha}s_G(n_g)}{\sqrt{n_g}}\right) \approx 1-\alpha \tag{2.4}$$

and hence that the CI formed by MRP will cover the optimality gap of $\hat{x}$ with the desired probability.

The lower bound given in (2.1) was independently introduced by Norkin et al. [47] and used for global optimization of stochastic programs within a branch-and-bound methodology. Other algorithmic work that uses Monte Carlo simulation-based bounds and multiple replications includes [1, 39]. MRP has been applied to different kinds of problems in the literature including a bond portfolio model [8], a stochastic vehicle routing problem [35] and supply chain network design [58].

There is other related work on assessing solution quality in stochastic programs via Monte Carlo methods, some being in the context of specific algorithms. Higle and Sen [27] derive a bound on the optimality gap for two-stage stochastic linear programs that is motivated by the Karush-Kuhn-Tucker optimality conditions; see also, Shapiro and Homem-de-Mello [60]. Higle and Sen [28] have also proposed a statistical lower bound that is rooted in duality. Dantzig and Infanger [18] and Higle and Sen [26, 30] use Monte Carlo versions of lower bounds obtained in sampling-based adaptations of deterministic cutting-plane algorithms.

2.2 Single Replication Procedure

When applying the multiple replications procedure reviewed above, the replication size is typically taken to be $n_g \geq 30$ in an attempt to have a valid statistical inference. This constitutes a drawback as one needs to solve at least 30 optimization problems (in step 1.2) in order to determine whether a candidate solution is of high quality. In this section, we show how a single replication, $n_g = 1$, can be used to make a valid statistical inference on the quality of a candidate solution.

As before, we assume that the candidate solution $\hat{x} \in X$ is given, and we use the following additional notation. For a feasible solution, $x \in X$, let $\bar{f}_n(x) = \frac{1}{n}\sum_{i=1}^{n} f(x, \tilde{\xi}^i)$, $\sigma^2_{\hat{x}}(x) = \text{var}[f(\hat{x}, \tilde{\xi}) - f(x, \tilde{\xi})]$ and $s^2_n(x) = \frac{1}{n-1}\sum_{i=1}^{n}[(f(\hat{x}, \tilde{\xi}^i) - f(x, \tilde{\xi}^i)) - (\bar{f}_n(\hat{x}) - \bar{f}_n(x))]^2$. Note that $G_n(\hat{x})$ given in equation (2.2) can be written as $\bar{f}_n(\hat{x}) - z^*_n$, with the understanding that the same n observations $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^n$ are used in $\bar{f}_n(\hat{x})$ and z^*_n. We define z_α to satisfy $P(N(0,1) \leq z_\alpha) = 1 - \alpha$. Below we state the single replication procedure (SRP).

SRP:

Input: Desired value of $0 < \alpha < 1$, sample size n and a candidate solution $\hat{x} \in X$.

Output: $(1-\alpha)$-level confidence interval on $\mu_{\hat{x}}$.

1. Sample i.i.d. observations $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^n$ from the distribution of $\tilde{\xi}$.

2. Solve (SP_n) to obtain x^*_n.

3. Calculate $G_n(\hat{x})$ as given in (2.2) and

$$s_n^2(x_n^*) = \frac{1}{n-1}\sum_{i=1}^{n}\left[(f(\hat{x},\tilde{\xi}^i) - f(x_n^*,\tilde{\xi}^i)) - (\bar{f}_n(\hat{x}) - \bar{f}_n(x_n^*))\right]^2.$$

4. Output one-sided CI on $\mu_{\hat{x}}$,

$$\left[0,\ G_n(\hat{x}) + \frac{z_\alpha s_n(x_n^*)}{\sqrt{n}}\right]. \tag{2.5}$$

The SRP differs from the MRP in that it uses a single replication and hence the sample variance is calculated differently. In the MRP, n_g i.i.d. observations of $G_n(\hat{x})$ are calculated and the sample variance of these gap estimates is used to form the CI. In contrast, only one value of $G_n(\hat{x})$ is calculated in SRP and the individual observations, $f(\hat{x},\tilde{\xi}^i) - f(x_n^*,\tilde{\xi}^i)$ for $i = 1,\ldots,n$, are used to calculate the sample variance. In fact, $G_n(\hat{x})$ is the sample mean of these individual observations and $s_n^2(x_n^*)$ is the corresponding sample variance. Below, we show how solving a single replication yields enough information to make a valid statistical inference concerning the quality of a candidate solution *even though* $G_n(\hat{x})$ may not be asymptotically normal. Before stating the theorem, we give the following proposition, which establishes consistency of the estimators. The proposition's hypothesis defines X^*, $x^*_{\min}$ and $x^*_{\max}$. In words, X^* denotes the set of optimum solutions and $x^*_{\min}$ and $x^*_{\max}$ are the optimal solutions to (SP) with minimum and maximum variance of $f(\hat{x},\tilde{\xi}) - f(x,\tilde{\xi})$, respectively.

Proposition 2.1. *Let* $X^* = \arg\min_{x\in X} Ef(x,\tilde{\xi})$, $x^*_{\min} \in \arg\min_{x\in X^*} \mathrm{var}[f(\hat{x},\tilde{\xi}) - f(x,\tilde{\xi})]$, *and* $x^*_{\max} \in \arg\max_{x\in X^*} \mathrm{var}[f(\hat{x},\tilde{\xi}) - f(x,\tilde{\xi})]$. *Assume (A1)-(A3),* $\hat{x} \in X$, *and that* $\tilde{\xi}^1,\tilde{\xi}^2,\ldots,\tilde{\xi}^n$ *are i.i.d. as* $\tilde{\xi}$. *Then,*

(i) $z_n^* \to z^*$, *w.p.1,*

(ii) all limit points of $\{x_n^*\}$ *lie in* X^*, *w.p.1,*

(iii) $\sigma^2_{\hat{x}}(x^*_{\min}) \leq \liminf_{n\to\infty} s_n^2(x_n^*) \leq \limsup_{n\to\infty} s_n^2(x_n^*) \leq \sigma^2_{\hat{x}}(x^*_{\max})$, *w.p.1.*

Proof. (A2) implies that $E\sup_{x\in X} f(x,\tilde{\xi}) < \infty$. Therefore, (i) follows immediately from Theorem A1 of [53, p.69]. (A1)-(A3) implies $\bar{f}_n(x)$ converges uniformly to $Ef(x,\tilde{\xi})$, w.p.1 on X. This coupled with (i) implies (ii). To prove (iii), we first show that the sequence of continuous functions $s_n^2(x)$ converges to $\sigma^2_{\hat{x}}(x)$ uniformly, w.p.1 on X. Let $g(x,\tilde{\xi}) = f(\hat{x},\tilde{\xi}) - f(x,\tilde{\xi})$. Then, with $\bar{g}_n(x) = \frac{1}{n}\sum_{i=1}^n g(x,\tilde{\xi}^i)$ we have

$$s_n^2(x) = \frac{n}{n-1}\left\{\frac{1}{n}\sum_{i=1}^n \Big(g(x,\tilde{\xi}^i) - Eg(x,\tilde{\xi})\Big)^2 - \Big(\bar{g}_n(x) - Eg(x,\tilde{\xi})\Big)^2\right\}.$$

The first term in the curly brackets is a sample mean of i.i.d. random variables and by Lemma A1 of [53, p.67] converges uniformly, w.p.1, to $\sigma^2_{\hat{x}}(x) = \operatorname{var} g(x,\tilde{\xi})$. Also, by the same lemma, $\bar{g}_n(x)$ converges uniformly to $Eg(x,\tilde{\xi})$, w.p.1, i.e., $\sup_{x\in X}\left|\bar{g}_n(x) - Eg(x,\tilde{\xi})\right| \to 0$, w.p.1. This implies

$$\sup_{x\in X}\Big(\bar{g}_n(x) - Eg(x,\tilde{\xi})\Big)^2 = \left(\sup_{x\in X}\left|\bar{g}_n(x) - Eg(x,\tilde{\xi})\right|\right)^2 \to 0, \text{ w.p.1.}$$

The sum of these two terms, $a_n(x) = \frac{1}{n}\sum_{i=1}^n (g(x,\tilde{\xi}^i) - Eg(x,\tilde{\xi}))^2 - (\bar{g}_n(x) - Eg(x,\tilde{\xi}))^2$, then converges uniformly to $\sigma^2_{\hat{x}}(x)$, w.p.1. To show uniform convergence of $\frac{n}{n-1}a_n(x)$, consider the following inequality

$$\sup_{x\in X}\left|a_n(x) + \frac{a_n(x)}{n-1} - \sigma^2_{\hat{x}}(x)\right| \leq \sup_{x\in X}\left|a_n(x) - \sigma^2_{\hat{x}}(x)\right| \quad + \quad \sup_{x\in X}\left|\frac{a_n(x) - \sigma^2_{\hat{x}}(x)}{n-1}\right| \quad + \quad \sup_{x\in X}\left|\frac{\sigma^2_{\hat{x}}(x)}{n-1}\right|.$$

By the above argument the first two terms on the right-hand side converge to 0, w.p.1. By (A2), $\sup_{x\in X} \sigma^2_{\hat{x}}(x) < \infty$. Thus, the last term also converges to 0, establishing uniform convergence.

Since X is compact, there exists a subsequence N along which $\{x^*_n\}_{n\in N}$ converges to a point in X, and by (ii) this point is in X^*, w.p.1. So, using the uniform convergence shown above,

$$\inf_{x\in X^*} \sigma^2_{\hat{x}}(x) \leq \lim_{\substack{n\to\infty \\ n\in N}} s^2_n(x^*_n) \leq \sup_{x\in X^*} \sigma^2_{\hat{x}}(x), \text{ w.p.1.}$$

The subsequence N is arbitrary and hence we obtain (iii). □

When (SP) has multiple optimum solutions, we cannot expect $\{x^*_n\}$ to have a unique limit point. However, by part (ii) of Proposition 2.1, all its limit points belong the set of optimum solutions, X^*. Similarly, $\{s^2_n(x^*_n)\}$ may not have a unique limit. That is why "lim inf" and "lim sup" appear in part (iii) of Proposition 2.1 instead of a "lim." Note that by (A2), $\sigma^2_{\hat{x}}(x^*_{\max}) < \infty$. When X^* is a singleton, $x^*_n \to x^*$, w.p.1 and $\liminf_{n\to\infty} s^2_n(x^*_n) = \limsup_{n\to\infty} s^2_n(x^*_n)$ $= \sigma^2_{\hat{x}}(x^*)$, w.p.1. We next present the main result regarding the validity of the SRP.

Theorem 2.2. *Assume (A1)-(A3), $\hat{x} \in X$, and that $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^n$ are i.i.d. as $\tilde{\xi}$. Given $0 < \alpha < 1$, for the SRP,*

$$\liminf_{n\to\infty} P\left(\mu_{\hat{x}} \leq G_n(\hat{x}) + \frac{z_\alpha s_n(x^*_n)}{\sqrt{n}}\right) \geq 1 - \alpha. \tag{2.6}$$

Proof. When $\hat{x} \in X^*$, inequality (2.6) is trivial. Suppose $\hat{x} \notin X^*$, and recall that $z_n^* = \min_{x \in X} \bar{f}_n(x)$. Thus,

$$G_n(\hat{x}) = \bar{f}_n(\hat{x}) - z_n^* \geq \bar{f}_n(\hat{x}) - \bar{f}_n(x), \quad \forall x \in X.$$

Replacing x by $x_{\min}^* \in \arg\min_{x \in X^*} \sigma_{\hat{x}}^2(x)$ we obtain,

$$\begin{aligned} & P\left(G_n(\hat{x}) + \frac{z_\alpha s_n(x_n^*)}{\sqrt{n}} \geq \mu_{\hat{x}}\right) \\ \geq \; & P\left(\bar{f}_n(\hat{x}) - \bar{f}_n(x_{\min}^*) + \frac{z_\alpha s_n(x_n^*)}{\sqrt{n}} \geq \mu_{\hat{x}}\right) \qquad (2.7) \\ = \; & P\left(\frac{(\bar{f}_n(\hat{x}) - \bar{f}_n(x_{\min}^*)) - \mu_{\hat{x}}}{\sigma_{\hat{x}}(x_{\min}^*)/\sqrt{n}} \geq -z_\alpha \frac{s_n(x_n^*)}{\sigma_{\hat{x}}(x_{\min}^*)}\right), \qquad (2.8) \end{aligned}$$

where in (2.8) we assume $\sigma_{\hat{x}}^2(x_{\min}^*) > 0$. Note that if $\sigma_{\hat{x}}^2(x_{\min}^*) = 0$ then $\mathrm{var}\,[\bar{f}_n(\hat{x}) - \bar{f}_n(x_{\min}^*)] = \frac{1}{n}\sigma_{\hat{x}}^2(x_{\min}^*) = 0$ and it follows from (2.7) that (2.6) is again trivial. Let $D_n = \frac{(\bar{f}_n(\hat{x}) - \bar{f}_n(x_{\min}^*)) - \mu_{\hat{x}}}{\sigma_{\hat{x}}(x_{\min}^*)/\sqrt{n}}$, $a_n = \frac{s_n(x_n^*)}{\sigma_{\hat{x}}(x_{\min}^*)}$ and $0 < \varepsilon < 1$, and for the moment assume $\alpha \leq 1/2$ so that $z_\alpha \geq 0$. Then (2.8) can be rewritten as

$$\begin{aligned} P\left(D_n \geq -z_\alpha a_n\right) \; & \geq \; P\left(D_n \geq -(1-\varepsilon)z_\alpha,\; a_n \geq 1-\varepsilon\right) \\ & = \; P\left(D_n \geq -(1-\varepsilon)z_\alpha\right) + P\left(a_n \geq 1-\varepsilon\right) - \\ & \quad\; P\left(\{D_n \geq -(1-\varepsilon)z_\alpha\} \cup \{a_n \geq 1-\varepsilon\}\right). \qquad (2.9) \end{aligned}$$

Taking limits we obtain,

$$\liminf_{n\to\infty} P\left(\mu_{\hat{x}} \leq G_n(\hat{x}) + \frac{z_\alpha s_n(x_n^*)}{\sqrt{n}}\right) \geq \Phi((1-\varepsilon)z_\alpha),$$

where Φ denotes the distribution function of the standard normal. By Proposition 2.1, the last two terms in (2.9) both converge to 1 and cancel out. Since $\bar{f}_n(\hat{x}) - \bar{f}_n(x_{\min}^*)$ is a sample mean of i.i.d. random variables, by the CLT the

first term in (2.9) converges to $\Phi((1-\varepsilon)z_\alpha)$. Letting ε shrink to zero gives the desired result, provided $\alpha \leq 1/2$. When $\alpha > 1/2$ we replace $x^*_{\min}$ with $x^*_{\max} \in \arg\max_{x \in X^*} \sigma^2_{\hat{x}}(x)$ in (2.8) and then use a straightforward variation of the above argument. $\square$

Theorem 2.2 justifies construction of the approximate $(1-\alpha)$-level one-sided confidence interval for $\mu_{\hat{x}} = Ef(\hat{x}, \tilde{\xi}) - z^*$, given in (2.5) without requiring $G_n(\hat{x}) = \bar{f}_n(\hat{x}) - z^*_n$ to be asymptotically normal. The intuitive reason for this is that minimization of the sample mean in z^*_n, while making asymptotic analysis of this random variable more difficult, projects the normal distribution so that the resulting confidence interval is conservative. This notion of projection is formalized in [53, Theorem 6.4.2] which states that scaled errors of z^*_n converge in distribution to the minimum of a collection of normal random variables. In other words, $\sqrt{n}(z^*_n - z^*) \Rightarrow \inf_{x \in X^*} Z(x)$, where each $Z(x)$ is a mean-zero normal random variable defined via $\sqrt{n}(\bar{f}_n(x) - z^*) \Rightarrow Z(x)$, $x \in X^*$. (Here, "$\Rightarrow$" denotes convergence in distribution.) If X^* is a singleton then $\inf_{x \in X^*} Z(x)$ is normally distributed. Otherwise, the precise nature of this random element is dictated by the dependency among $Z(x)$ for $x \in X^*$. We note that because we estimate the sample variance in the SRP, we recommend the more conservative Student's t-quantiles, $t_{n-1,\alpha}$, when n is small.

We reviewed a procedure in which we use $n_g \geq 30$ replications and then introduced a procedure with just one replication, $n_g = 1$. Even though the single replication procedure is computationally significantly less demanding,

solving a single minimization problem might also create some difficulties. For instance, in step 2 of the procedure, if the minimization problem used to calculate the gap estimate yields a solution x_n^* that is equal to $\hat{x}$, then both the gap estimate $G_n(\hat{x})$ and the variance estimate $s_n^2(x_n^*)$ are zero and consequently the CI on the optimality gap given in (2.5) has width zero. For small sample sizes, this can happen even though the candidate solution $\hat{x}$ is far from optimal. (Proposition 2.1 eliminates this possibility as the sample size grows large.) The following example illustrates this effect.

Example 2.1. *Consider the following problem,* $\{\min E[\tilde{\xi}x] : -1 \leq x \leq 1\}$, *where* $\tilde{\xi} \sim N(\mu, 1)$ *and* $\mu > 0$. *Note that (A1)-(A3) are satisfied. The optimal solution to this problem is* $x^* = -1$ *and the candidate solution* $\hat{x} = 1$ *has the largest optimality gap of* $\mu_{\hat{x}} = 2\mu$. *Suppose we use the SRP with* $\alpha = 0.10$ *and* $n = 50$ *for the candidate solution* $\hat{x} = 1$. *When the random sample has* $\bar{\xi} = \frac{1}{n}\sum_{i=1}^{n} \tilde{\xi}^i < 0$, *then* $x_n^* = 1$ *and* $G_n(\hat{x}) = s_n(x_n^*) = 0$. *Hence, for the problem instance with* $\mu = 0.1$, *the coverage probability* $P\left(\mu_{\hat{x}} \leq G_n(\hat{x}) + z_\alpha s_n(x_n^*)/\sqrt{n}\right) \leq 1 - P(\bar{\xi} < 0) \simeq 0.760$ *is below the desired level of* 0.90 *when a sample size of* $n = 50$ *is used.*

This effect can be lessened by using a larger sample size or by performing more than one replication. The ideas used to show the validity of the single replication procedure can also be used to justify use of procedures with a small number of replications. In the next section, we focus on procedures with two replications.

2.3 Two-Replication Procedures

In this section we develop two procedures to assess solution quality in stochastic programs that use two replications. The first one, which we call the independent 2-replication procedure (I2RP), aims to eliminate the correlation between $G_n(\hat{x})$ and $s_n(x_n^*)$, by performing two independent replications, one to estimate the gap and the other to estimate $s_n(x_n^*)$.

I2RP:

Recall the definition of the SRP and replace step 3 by:

3′. Calculate $G_n^1(\hat{x})$ as given in (2.2) and to calculate the sample variance

3′.1. Sample i.i.d. observations $\tilde{\xi}^{n+1}, \ldots, \tilde{\xi}^{2n}$ from the distribution of $\tilde{\xi}$,

3′.2. Solve (SP_n) defined with respect to $\tilde{\xi}^{n+1}, \ldots, \tilde{\xi}^{2n}$ to obtain x_n^{2*},

3′.3. Calculate $s_n^2(x_n^{2*}) = \frac{1}{n-1}\sum_{i=1}^{n}[(f(\hat{x}, \tilde{\xi}^{n+i}) - f(x_n^{2*}, \tilde{\xi}^{n+i})) - (\bar{f}_n(\hat{x}) - \bar{f}_n(x_n^{2*}))]^2$, where the sample means in this sample variance computation are also with respect to the second sample.

The confidence interval on the optimality gap is formed exactly as in (2.5), where the gap point estimate, $G_n^1(\hat{x})$, comes from the first replication and the sample standard deviation, $s_n(x_n^{2*})$, comes from the second replication. Even though I2RP requires twice the computational effort compared to a single replication procedure, the correlation between these two estimates becomes zero. Following the ideas in the proof of Theorem 2.2, it can easily be shown

that this procedure provides an asymptotically valid confidence interval. We formally state this in the theorem below.

Theorem 2.3. *Assume (A1)-(A3), $\hat{x} \in X$, and that $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^{2n}$ are i.i.d. as $\tilde{\xi}$. Given $0 < \alpha < 1$, for the I2RP,*

$$\liminf_{n\to\infty} P\left(\mu_{\hat{x}} \leq G_n^1(\hat{x}) + \frac{z_\alpha s_n(x_n^{2*})}{\sqrt{n}}\right) \geq 1 - \alpha.$$

Proof. The proof of Theorem 2.2 remains the same when $s_n^2(x_n^*)$ is redefined as in step 3′. □

A natural extension of the I2RP is to use all the information available from the two replications. In other words, we have a single sample of size $2n$ and partition it (randomly) into two sets of size n. In each set we perform the SRP and average the two estimates. We call this the averaged two-replication procedure (A2RP).

A2RP:

Recall the definition of the MRP and fix $n_g = 2$. Replace steps 1.3, 2 and 3 by:

1.3′. Calculate $G_n^i(\hat{x})$ and $s_n^2(x_n^{i*})$.

2′. Calculate the estimates by taking the average,

$$G_n'(\hat{x}) = \frac{1}{2}\left(G_n^1(\hat{x}) + G_n^2(\hat{x})\right) \quad \text{and} \quad s_n^{2\prime} = \frac{1}{2}\left(s_n^2(x_n^{1*}) + s_n^2(x_n^{2*})\right). \tag{2.10}$$

3′. Output one-sided CI on $\mu_{\hat{x}}$,

$$\left[0,\ G_n'(\hat{x}) + \frac{z_\alpha s_n'}{\sqrt{2n}}\right].$$

Unlike the MRP, the sample variance, $s_n^2(x_n^{i*})$, for each sample $i = 1, 2$, is calculated as in the single replication procedure (in step 1.3′) and these are averaged to obtain the variance estimator of the A2RP (in step 2′). This variance estimator given in (2.10) is a pooled estimator, similar in spirit to that used in a two-sample t-test for testing the difference of means from populations with equal variance [12, p.396]. It is a consistent estimator, in the sense that $\sigma_{\hat{x}}^2(x_{\min}^*) \leq \liminf_{n\to\infty} s_n^{2\prime} \leq \limsup_{n\to\infty} s_n^{2\prime} \leq \sigma_{\hat{x}}^2(x_{\max}^*)$, w.p.1, by Proposition 2.1. A2RP provides an asymptotically valid CI on the optimality gap, as stated in the theorem below.

Theorem 2.4. *Assume (A1)-(A3), $\hat{x} \in X$, and that $\tilde{\xi}^{i1}, \tilde{\xi}^{i2}, \ldots, \tilde{\xi}^{in}$, $i = 1, 2$, are i.i.d. as $\tilde{\xi}$. Given $0 < \alpha < 1$, for the A2RP,*

$$\liminf_{n\to\infty} P\left(\mu_{\hat{x}} \leq G_n'(\hat{x}) + \frac{z_\alpha s_n'}{\sqrt{2n}}\right) \geq 1 - \alpha.$$

Proof. With an obvious extension of notation to index each sample, we have

$$\bar{f}_n^1(\hat{x}) - z_n^{1*} \geq \bar{f}_n^1(\hat{x}) - \bar{f}_n^1(x_{\min}^*) \qquad \text{and} \qquad \bar{f}_n^{\,2}(\hat{x}) - z_n^{2*} \geq \bar{f}_n^2(\hat{x}) - \bar{f}_n^2(x_{\min}^*). \tag{2.11}$$

Multiplying each of the inequalities in (2.11) by 1/2 and summing, we obtain

$$\begin{aligned} G_n'(\hat{x}) &\geq \frac{1}{2}\left([\bar{f}_n^1(\hat{x}) - \bar{f}_n^1(x_{\min}^*)] + [\bar{f}_n^2(\hat{x}) - \bar{f}_n^2(x_{\min}^*)]\right) \\ &= \bar{f}_{2n}(\hat{x}) - \bar{f}_{2n}(x_{\min}^*). \end{aligned}$$

Since $\bar{f}_{2n}(\hat{x}) - \bar{f}_{2n}(x^*_{\min})$ is a sample mean of i.i.d. random variables, by the CLT, $\sqrt{2n}((\bar{f}_{2n}(\hat{x}) - \bar{f}_{2n}(x^*_{\min})) - \mu_{\hat{x}})$ converges in distribution to a normal random variable with mean zero and variance $\sigma^2_{\hat{x}}(x^*_{\min})$. Also, $\liminf_{n\to\infty} \frac{s'_n}{\sigma_{\hat{x}}(x^*_{\min})} \geq 1$, w.p.1, by Proposition 2.1. The rest of the proof for $\alpha \leq 1/2$ case is analogous to that of Theorem 2.2, and the proof for $\alpha > 1/2$ is again straightforward. □

Note that the independent two-replication procedure uses $\sqrt{n}$ as the scaling factor whereas the averaged two-replication procedure uses $\sqrt{2n}$. Even though the two procedures use the same number of observations, the A2RP uses all of the information to form both estimators whereas I2RP uses half of the information for each estimator. However, I2RP eliminates the correlation between the gap and variance estimators. Now let us turn back to Example 2.1 to illustrate the two-replication procedures.

Example 2.2. *Consider the specific problem instance given in Example 2.1. Let* $\bar{\xi}_1 = \frac{1}{n}\sum_{i=1}^{n} \tilde{\xi}^i$ *be the sample mean of the first sample and likewise,* $\bar{\xi}_2$ *be the sample mean of the second sample. With* $\mu = 0.1$ *and* $n = 50$*, the probability of obtaining a CI of width 0 from I2RP or A2RP is* $P(\bar{\xi}_1 < 0)P(\bar{\xi}_2 < 0) = 0.057$*, from normal quantiles. Therefore, for the two-replication procedures that use a sample size of* $n = 50$ *for each replication, the coverage probabilities are bounded above by* 0.943*, compared to* 0.760 *for SRP in Example 2.1. For SRP that uses a sample size of* $2n = 100$*, the upper bound for the coverage probability is* 0.841*.*

2.4 Empirical Coverage Results

In this section, we empirically analyze the small-sample behavior of the described procedures. Theorems 2.2, 2.3 and 2.4 show that the confidence intervals formed using the three procedures, SRP, I2RP and A2RP are asymptotically valid. In other words, these theorems establish that the CIs have the desired coverage probability as the sample size grows large ($n \to \infty$). Example 2.1 suggests that this might not hold for SRP for small values of n. To investigate how the procedures behave for small sample sizes, in this section we first apply them to a newsvendor problem under uniform demand and then to three small two-stage stochastic linear programs from the literature and compare empirical coverage probabilities.

The output of our procedures is a confidence interval on the optimality gap. In this section, we report yet another confidence interval, namely, a CI on the coverage probability associated with our procedures' output for various values of n. For more details on this, refer to Chapter 1, Section 1.2. We briefly explain our experiments. To perform the tests, we set $\alpha = 0.10$ and repeat the procedures k times for varying values of sample sizes, n. For a given value of n, we form $\hat{p}_n$, the fraction of the k repetitions in which the CI contains the true gap. Quantity $\hat{p}_n$ is an estimator of the true coverage probability p_n. Ideally, we would like to have $p_n \geq 1 - \alpha = 0.90$. Recall that $\hat{p}_n$ is a (scaled) binomial random variable and for sufficiently large values of k, we can use the CLT to form a 90% confidence interval on the true coverage probability via $\hat{p}_n \pm 1.645(\hat{p}_n(1 - \hat{p}_n)/k)^{1/2}$. In the tables that follow, we report this interval.

In order to lessen the effect of variation in the samples, for each sample size n, we use the same observations from the SRP to form CIs for I2RP and A2RP. In other words, we compare SRP with sample size n with two-replication procedures that use the same n observations and a random partition of these observations into two samples of size $n/2$. For MRP, we set the number of replications $n_g = 30$ and typically take k smaller than the single or two-replication procedures as the computational requirement is higher. To understand how the estimator $s_n(x_n^*)$ affects coverage, we form another CI by taking $G_n(\hat{x})$ from SRP and replacing $s_n(x_n^*)$ by $\sigma_{\hat{x}}(x^*)$ in (2.5). We denote this procedure as TRUE. We now turn to the computational results for the test problems.

2.4.1 Newsvendor Problem

The newsvendor problem is a classical example of a stochastic program with simple recourse and its properties are well known, e.g., [9, p.15]. We briefly review its formulation. Let r be the selling price of a newspaper, $0 < c < r$ be its cost to the vendor, and $\tilde{\xi}$ denote the nonnegative random demand. The vendor's problem is to find the number of papers to buy, x, so that the expected profit is maximized. So, the problem is formulated as $\max\left\{-cx + rE\min\{x,\ \tilde{\xi}\} : x \geq 0\right\}$ and its solution is given by x^* that solves $\inf_{x\geq 0} P(\tilde{\xi} \leq x) \geq (r-c)/r$, which is simply $\int_0^{x^*} dF(\xi) = (r-c)/r$, when the demand distribution is continuous with distribution function F. Note that the newsvendor problem is of the form (SP) with $f(x, \tilde{\xi}) = cx - r\min\{x,\ \tilde{\xi}\}$ and

n	MRP	SRP	I2RP	A2RP	TRUE
50	0.9873 ± 0.0018	0.8756 ± 0.0017	0.9421 ± 0.0012	0.9273 ± 0.0012	0.9530 ± 0.0011
100	0.9741 ± 0.0026	0.8895 ± 0.0016	0.9299 ± 0.0013	0.9106 ± 0.0013	0.9360 ± 0.0013
200	0.9594 ± 0.0032	0.8898 ± 0.0016	0.9290 ± 0.0013	0.9124 ± 0.0013	0.9249 ± 0.0014
300	0.9483 ± 0.0036	0.8946 ± 0.0016	0.9257 ± 0.0014	0.9106 ± 0.0014	0.9188 ± 0.0014
400	0.9390 ± 0.0039	0.8944 ± 0.0016	0.9180 ± 0.0014	0.9061 ± 0.0014	0.9165 ± 0.0014
500	0.9359 ± 0.0040	0.8937 ± 0.0016	0.9192 ± 0.0014	0.9066 ± 0.0014	0.9140 ± 0.0015
600	0.9350 ± 0.0041	0.8962 ± 0.0016	0.9187 ± 0.0014	0.9079 ± 0.0014	0.9143 ± 0.0015
700	0.9299 ± 0.0042	0.8960 ± 0.0016	0.9153 ± 0.0014	0.9048 ± 0.0014	0.9124 ± 0.0015
800	0.9287 ± 0.0042	0.8959 ± 0.0016	0.9139 ± 0.0015	0.9058 ± 0.0015	0.9123 ± 0.0015
900	0.9317 ± 0.0041	0.8970 ± 0.0016	0.9146 ± 0.0015	0.9061 ± 0.0014	0.9118 ± 0.0015
1000	0.9267 ± 0.0043	0.8970 ± 0.0016	0.9143 ± 0.0015	0.9048 ± 0.0014	0.9105 ± 0.0015

Table 2.1: Empirical coverage results, $\hat{p}_n \pm 1.645(\hat{p}_n(1-\hat{p}_n)/k)^{1/2}$, for various values of n, where k =10,000 for MRP and 100,000 for SRP, I2RP, A2RP and TRUE. Confidence intervals for TRUE are calculated by using $G_n(\hat{x})$ from SRP and replacing $s_n(x_n^*)$ by $\sigma_{\hat{x}}(x^*)$ in (2.5).

$X = \{x : x \geq 0\}$.

We assume $\tilde{\xi} \sim U(0, b),\ b > 0$ and hence modify X to $\{x : 0 \leq x \leq b\}$. Note that (A1)-(A3) hold. To perform the tests, we set $\alpha = 0.10$. For the problem parameters, we use $c = 5$, $r = 15$ and $b = 10$. This problem has optimal solution $x^* = 6\frac{2}{3}$ with expected profit $z^* = 33\frac{1}{3}$. For the candidate solution $\hat{x}$, we pick a solution that has expected profit 10% from the optimum. We use $\hat{x} = 8.775$ with $Ef(\hat{x}, \tilde{\xi}) = 30$ and with an optimality gap of $\mu_{\hat{x}} = 3\frac{1}{3}$. This candidate solution has $\sigma^2_{\hat{x}}(x^*) = 140.79$. For the SRP, I2RP, A2RP and TRUE we construct k =100,000 confidence intervals and for the MRP, we construct k =10,000 intervals for each value of the sample size. We take sample sizes, n, between 50 and 1,000. Table 2.1 summarizes the results. For example, when n =1,000, for the MRP, the table indicates $\hat{p}_n = 0.9267$ so that we are confident at level 0.90 that the true coverage probability, i.e., the

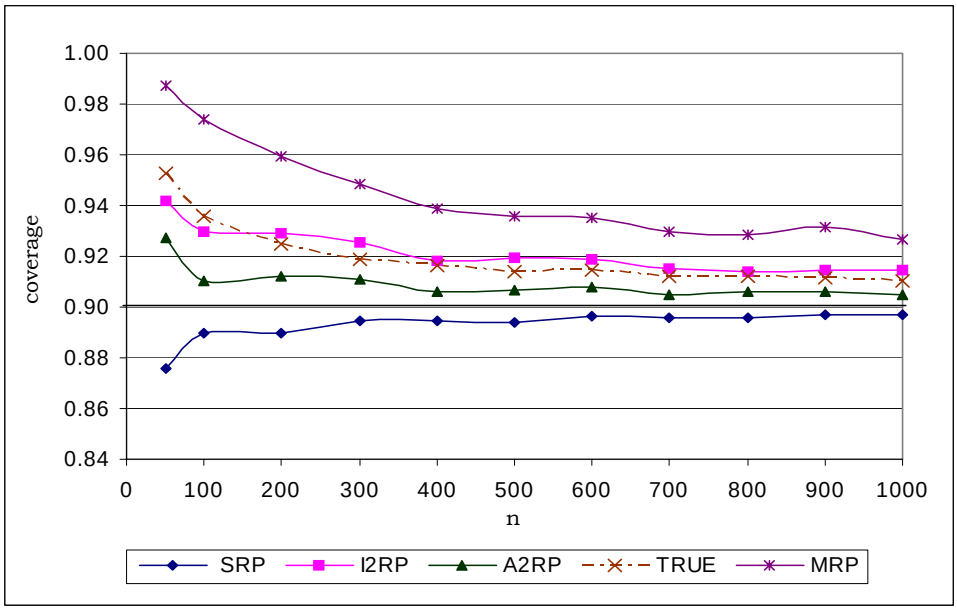

Figure 2.1: Empirical coverage probability ($\hat{p}_n$) versus sample size (n) for the newsvendor problem.

left-hand side of (2.4), is in $[0.9224, 0.9310]$.

Figure 2.1 shows a plot of $\hat{p}_n$ versus n for each of the procedures. The coverage for the MRP exceeds the desired coverage of 90% but shrinks toward 90% as the sample size increases. The bias, $Ez_n^* - z^*$, constitutes a major part of the CI formed by MRP and thus this CI tends to overestimate the optimality gap. As indicated in Section 2.1, the bias shrinks as n increases and the coverage of MRP falls as n grows. The SRP, on the other hand, has slightly less than the desired coverage of 90%. Even though the bias is larger when the sample size is small, the number of times a single replication CI contains the optimality gap approaches 90% from below. With a more careful

Problem	$\hat{x}$	$Ef(\hat{x}, \tilde{\xi})$	$\mu_{\hat{x}}$	$\sigma_{\hat{x}}(x^*)$
CEP1	$(0, 125, 875, 2500,$ $0, 625, 1375, 3000)$	393,288.01	38,129.09	55,690.34
PGP2	$(1.5, 5.5, 5, 4.5)$	448.46	1.14	82.69
APL1P	$(1111.11, 2300)$	24,807.16	164.84	1,893.03

Table 2.2: Candidate solutions used in tests.

n	MRP	SRP	I2RP	A2RP	TRUE
50	0.860 ± 0.057	0.912 ± 0.021	0.912 ± 0.021	0.920 ± 0.020	0.928 ± 0.019
100	0.940 ± 0.039	0.888 ± 0.023	0.898 ± 0.022	0.890 ± 0.023	0.912 ± 0.021
150	0.910 ± 0.047	0.912 ± 0.021	0.926 ± 0.019	0.906 ± 0.021	0.918 ± 0.020
200	0.920 ± 0.045	0.894 ± 0.023	0.906 ± 0.021	0.894 ± 0.023	0.906 ± 0.021

Table 2.3: Empirical coverage results for CEP1.

examination, we see a similar effect as illustrated in Example 2.1. For small sample sizes, $G_n(\hat{x})$ is more variable and we have observed from the individual replications that when it is small, $s_n(x_n^*)$ also tends to be small, resulting in a narrow CI width. In particular, this happens when x_n^* is close to $\hat{x}$, even though $\hat{x}$ is not close to x^*. The two-replication procedures lessen this effect by using two samples and two estimates $x_{n/2}^*$. For this instance of the newsvendor problem, their coverage probabilities approach 90% from above.

2.4.2 Two-Stage Stochastic Linear Programs

In this section, we apply the procedures to three two-stage stochastic linear programs with recourse from the literature. The first one, denoted CEP1, is a capacity expansion planning problem with random demand. The dimension of the random vector $\tilde{\xi}$ for CEP1 is 3 and it has 216 total realizations. The second test problem, PGP2, is an electric power generation model,

again with 3 stochastic parameters but with 576 realizations. Both CEP1 and PGP2 are described in [29, pp. 3-10]. The third test problem we use, denoted APL1P, can be found in [33]. It is a power expansion planning problem where $\tilde{\xi}$ has 5 independent elements and 1280 realizations. Since these test problems have small numbers of realizations, it is possible to calculate true optimality gaps and variances. Table 2.2 lists the candidate solutions we use for each problem. For example, the dimension of the candidate solution $\hat{x}$ for CEP1 is 8 and this candidate solution is approximately 10.7% ($= 100 \times \mu_{\hat{x}}/z^*$) from the optimal.

To solve the sampling problems, we used the regularized decomposition algorithm of [55]. An accelerated implementation of this algorithm is in C++ [57] and we have modified this code to perform the tests. For each test problem under SRP, I2RP, A2RP and TRUE, we construct $k = 500$ confidence intervals for various values of the sample size n. For MRP, we use $n_g = 30$ and construct $k = 100$ confidence intervals for the same values of n. Tables 2.3, 2.4 and 2.5 list results for CEP1, PGP2 and APL1P, respectively. As PGP2 and APL1P have high variance relative to the optimality gap, the sampling error term in the CI for TRUE, i.e., $z_\alpha \sigma_{\hat{x}}(x^*)/\sqrt{n}$, dominates and results in mostly 100% coverage. Similarly, the MRP, while computationally more expensive than the single and two-replication procedures is largely conservative with respect to its coverage results.

For CEP1 the optimal solution, x^*, is quite easy to find by a sampling problem. That is, the probability that x_n^* equals x^* is quite high even for small

n	MRP	SRP	I2RP	A2RP	TRUE
50	1 ± 0	0.536 ± 0.037	0.708 ± 0.033	0.876 ± 0.024	1 ± 0
100	1 ± 0	0.572 ± 0.036	0.676 ± 0.034	0.766 ± 0.031	1 ± 0
200	1 ± 0	0.472 ± 0.037	0.792 ± 0.030	0.806 ± 0.029	1 ± 0
300	1 ± 0	0.662 ± 0.035	0.810 ± 0.029	0.906 ± 0.021	1 ± 0
400	1 ± 0	0.578 ± 0.036	0.712 ± 0.033	0.730 ± 0.033	1 ± 0
500	1 ± 0	0.504 ± 0.037	0.854 ± 0.026	0.864 ± 0.025	1 ± 0

Table 2.4: Empirical coverage results for PGP2.

sample sizes. Therefore, CEP1 seems to have fairly good coverage for each of the procedures. In contrast, both PGP2 and APL1P yield different solutions, x_n^*, to sampling problems for values of n we consider. In fact, for PGP2 we have observed that the optimal solution x^* and the candidate solution given in Table 2.2 each appear as x_n^* almost 45% of the time when $n = 500$. Thus, due to the same effect illustrated in Example 2.1, the coverage results for this candidate solution are very low. Two-replication procedures have higher coverage compared to SRP but are still below the desired level of 90%. For APL1P, we have observed that the probability of obtaining x^* as x_n^* is even lower than PGP2. However, x_n^* takes a variety of different values for APL1P's sampling problems, compared to predominantly two distinct values for PGP2. Thus, the resulting coverage results are good for larger sample sizes for SRP and the two-replication procedures perform well even for small sample sizes.

2.5 Further Analysis and Preliminary Guidelines

As illustrated in Example 2.1 and the computational results of the previous section, in some problems the nature of the candidate solution $\hat{x}$ and

n	MRP	SRP	I2RP	A2RP	TRUE
50	1 ± 0	0.782 ± 0.030	0.940 ± 0.017	0.932 ± 0.019	1 ± 0
100	1 ± 0	0.786 ± 0.030	0.910 ± 0.021	0.918 ± 0.020	1 ± 0
200	1 ± 0	0.828 ± 0.028	0.908 ± 0.021	0.902 ± 0.022	1 ± 0
300	1 ± 0	0.832 ± 0.028	0.918 ± 0.020	0.880 ± 0.024	1 ± 0
400	1 ± 0	0.850 ± 0.026	0.928 ± 0.019	0.886 ± 0.023	0.992 ± 0.007
500	1 ± 0	0.902 ± 0.022	0.940 ± 0.017	0.908 ± 0.021	0.966 ± 0.013
600	1 ± 0	0.894 ± 0.023	0.944 ± 0.017	0.910 ± 0.021	0.968 ± 0.013
700	1 ± 0	0.910 ± 0.021	0.964 ± 0.014	0.934 ± 0.018	0.966 ± 0.013
800	1 ± 0	0.910 ± 0.021	0.962 ± 0.014	0.934 ± 0.018	0.962 ± 0.014
900	1 ± 0	0.906 ± 0.021	0.965 ± 0.014	0.934 ± 0.018	0.948 ± 0.016
1000	1 ± 0	0.906 ± 0.021	0.956 ± 0.015	0.926 ± 0.019	0.956 ± 0.015

Table 2.5: Empirical coverage results for APL1P.

the solution(s) x_n^* used in our procedures can lead to inferior performance of the procedures. In particular, the procedures can work poorly when $\hat{x} \notin X^*$ is chosen to be a candidate solution from an auxiliary sampling problem and this solution has a high probability of occurrence as an x_n^* solution to an (SP_n) used in our procedures. In such cases, especially the SRP can report a CI width which is too narrow, over-stating the quality of the candidate solution. Two-replication procedures reduce this effect, but they may not be enough. Let us return to the problem discussed in Examples 2.1 and 2.2 and show that for a fixed value of n, however large, the two-replication procedures can have low coverage.

Example 2.3. *For the problem discussed in Examples 2.1 and 2.2, as* $\mu \to 0$*, the upper bound on the coverage probability, i.e.,* $1 - P($*obtaining a CI of width 0*$)$*, for SRP approaches* 0.50 *and the same upper bound for I2RP and A2RP approaches* 0.75 *for all sample sizes. Note that for a fixed* μ*, we obtain*

$(1-\alpha)$-level coverage as $n \to \infty$. However, for a fixed n we obtain 0.50-level coverage for the SRP and 0.75-level coverage for the two-replication procedures as $\mu \to 0$.

One alternative is to employ the more conservative multiple replications procedure, MRP. Another option is to average more than two replications, again at the expense of solving more optimization problems. For instance A3RP, the three-replication variant of A2RP, will increase the upper bound on the coverage probability from 0.75 to 0.875 as $\mu \to 0$ in Example 2.3.

Let us now examine PGP2 in more detail to gain more insight. Table 2.6 lists the most frequent x_n^* solutions to 10,000 sampling problems of size $n = 500$ for PGP2. We also report empirical coverage probabilities when taking each of these as the candidate solution under $k = 500$ repetitions of the SRP, again for a sample size of $n = 500$. The optimal solution, x^*, and the candidate solution used in the previous section, x_1, each appear approximately 45% of the time. Points x_1 and x_2 are quite close to each other (in terms discussed in more detail below) and they both result in very low coverage of the SRP. When $\hat{x} = x_1$ or x_2 and either of these points happens to solve the sampling problem in SRP, the resulting CI width is zero or nearly zero, lowering the coverage probability.

We say two points $x', x'' \in X$ coincide if $\text{var}[f(x', \tilde{\xi}) - f(x'', \tilde{\xi})] = 0$ and that they nearly coincide if this variance is small. This occurs if $x' = x''$ but it can also occur when x' and x'' are distinct. When a candidate solution $\hat{x}$

nearly coincides with a high probability $x_n^* \notin X^*$, the gap random variable is nearly degenerate and we can have undercoverage. So, even though x_2 from Table 2.6 has a relatively low probability of occurrence, it nearly coincides with the higher probability x_1, leading to low coverage.

x_i		Frequency	$Ef(x_i, \tilde{\xi})$	μ_{x_i}	Coverage
$x^* = x_0$	(1.5, 5.5, 5, 5.5)	44.49%	447.324	0	1 ± 0
x_1	(1.5, 5.5, 5, 4.5)	43.90%	448.464	1.140	0.504 ± 0.037
x_2	(1.5, 5, 5, 5)	4.44%	448.511	1.186	0.504 ± 0.037
x_3	(1.5, 5.5, 5, 5)	3.54%	447.752	0.428	0.946 ± 0.017
x_4	(1.5, 5, 5, 6)	1.56%	447.376	0.051	0.970 ± 0.013

Table 2.6: Solutions to 10,000 (SP_{500}) for PGP2. We report coverage of SRP out of 500 repetitions for sample size of $n = 500$.

2.5.1 ε-Optimal Solutions

In this section, we consider an approach based on ε-optimal solutions to help avoid $\hat{x}$ and x_n^* coinciding. While $\hat{x}$ can be generated by any method, typically, $\hat{x}$ may be obtained by solving a sample-mean problem with sample size $n_{\hat{x}}$, ($\text{SP}_{n_{\hat{x}}}$). Then, we assess its quality via SRP by solving a separate (SP_n). Here, $n_{\hat{x}}$ and n could be the same or differ (typically $n_{\hat{x}} \geq n$) and the same holds for the two "epsilons" used when approximately solving ($\text{SP}_{n_{\hat{x}}}$) and (SP_n). There are clearly a number of possibilities but since our focus is on assessing solution quality, we use ε-optimal solutions when solving (SP_n) for the SRP. We believe solving (SP_n) approximately makes sense, particularly in light of the fact that our procedure's output is a confidence interval. Similarly,

we can use ε-optimal solutions for the two sampling problems used in I2RP and A2RP.

For our computational results, as before, we used the regularized decomposition (RD) code of [57]. This is similar to the multicut version of the L-Shaped method [10], except that the master problem has a regularizing proximal term. The quadratic proximal term can result in considerable computational savings. Because of the regularizing term, the objective function value of the master problem in RD does not provide a lower bound on the problem's optimal value. So, we first run RD with the proximal term and then remove the proximal term in order to obtain a lower bound on z_n^*. When this procedure terminates, we have $\underline{z}_n^* \leq z_n^* \leq \overline{z}_n^*$. If we solve the problem with sufficient precision, $\underline{z}_n^* = z_n^* = \overline{z}_n^*$. However, in this section we solve the sampling problem (SP_n) with varying degrees of suboptimality, and use the lower bound, $\underline{z}_n^*$, for constructing the gap and the sampling variance estimates.

We applied this methodology to the two candidate solutions, x_1 and x_2 of PGP2, which have poor coverage results, using SRP, I2RP and A2RP. Figures 2.2 and 2.3 show the results of our computations. On the y-axis, we plot the empirical coverage probability of the procedures out of $k = 500$ repetitions for a sample size of $n = 500$. On the x-axis, we plot the suboptimality with which we solved the sampling problems (SP_n) to obtain the confidence interval estimators. Suboptimality is measured as $(\overline{z}_n^* - \underline{z}_n^*)/\min\{|\overline{z}_n^*|, |\underline{z}_n^*|\}$. The vertical dashed line in the figures is the ratio of the optimality gap of the candidate solution to the optimum value of PGP2, $\mu_{\hat{x}}/z^*$. This value is 2.5×10^{-3} for

$\hat{x} = x_1$ and 2.7×10^{-3} for $\hat{x} = x_2$. Even though this is measured with respect to z^* and the suboptimality is measured with respect to z_n^*, we expect to have almost 100% coverage after this point. However, all of the procedures reach the desired level of coverage earlier than this, for a suboptimality of around 1.5×10^{-3}. The two-replication procedures reach the desired coverage of 0.90 at a suboptimality of 1×10^{-3}.

2.5.2 Preliminary Guidelines

So far, we have presented several computationally attractive alternatives to the MRP for assessing solution quality in stochastic programs. That said, in certain cases, we recommend the use of MRP instead of SRP or one of the two-replication procedures. Below we summarize our preliminary guidelines on which method to use.

- If computation is quite cheap, we recommend the more conservative MRP.
- If the desire for conservative coverage results is paramount, we again recommend MRP.
- Otherwise, among the small replication procedures, we recommend using A2RP with ε-optimal solutions, based on our computational experience to date.

Relative to the SRP, the two-replication procedures help to avoid $\hat{x}$ and x_n^* coinciding and hence improve coverage results. The use of ε-optimal solutions further assist in improving coverage results for two reasons. First,

like the two-replication procedures, the likelihood of coinciding solutions is reduced. Second, our use of lower bounds $\underline{z}_n^*$ in place of z_n^* when solving (SP_n) suboptimally has the effect of inflating the confidence interval width. In our preliminary computations, small suboptimality levels (e.g., 0.10%-0.20%) were enough to reach the desired level of coverage. Finally, we note that relative to I2RP, the A2RP uses all of the observations in both the point estimate of the gap and the sampling-error estimate. Empirically, this advantage appears to come without detrimental effects on coverage.

2.6 Concluding Remarks

In this chapter, we have developed Monte Carlo sampling-based procedures for assessing solution quality in stochastic programs. Compared to an earlier multiple replications procedure that requires solution of at least 30 optimization problems, the methods we introduce require solution of one or two optimization problems. An illustrative example and computational results substantiate that when a solution $\hat{x} \notin X^*$ to an auxiliary sampling problem (SP_n) is chosen as the candidate solution, and this solution has a high probability of occurring as the x_n^* used in the SRP, the coverage probability can be quite low. So, we develop variants of this procedure that use two replications to lessen this effect. With the same motivation, we have proposed using ε-optimal solutions when solving the sampling problem (SP_n) used in our confidence interval estimation procedures. Our computational results seem to indicate that at quite modest values of suboptimization, this approach can

work well.

Among the small replication procedures, we recommend the use of A2RP with ε-solutions. MRP is the most conservative of all our methods and may be preferred if computations are cheap, or, if conservative coverage results are desired. We note that the sample variance estimator of the small replication procedures is different than that of the MRP. When the sampling error dominates the point estimate of (the bound on) the optimality gap, the resulting CI could be quite large. In the next chapter, we examine sequential methods for assessing solution quality that are designed to control this sampling error.

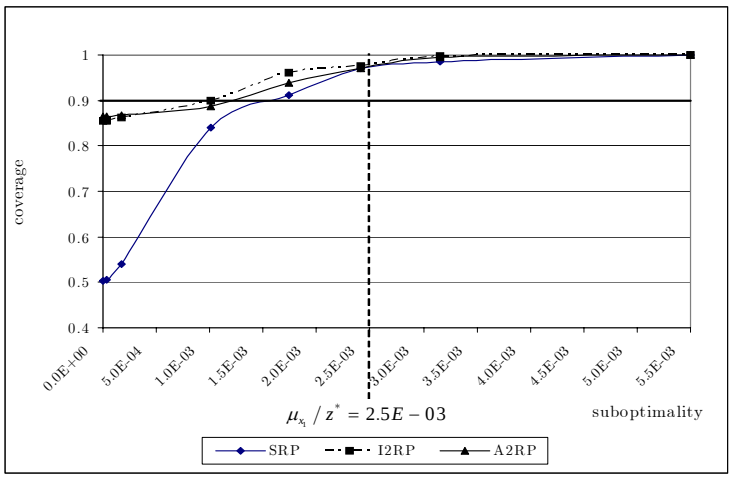

Figure 2.2: We plot the empirical coverage probability out of $k = 500$ repetitions with sample size $n = 500$ for the candidate solution $\hat{x} = x_1$ of PGP2. We solved the sampling problem(s) (SP_n) in the estimation of SRP (I2RP, A2RP) with varying level of suboptimality. The vertical dashed line represents the ratio of the optimality gap of x_1 to the optimal value of PGP2.

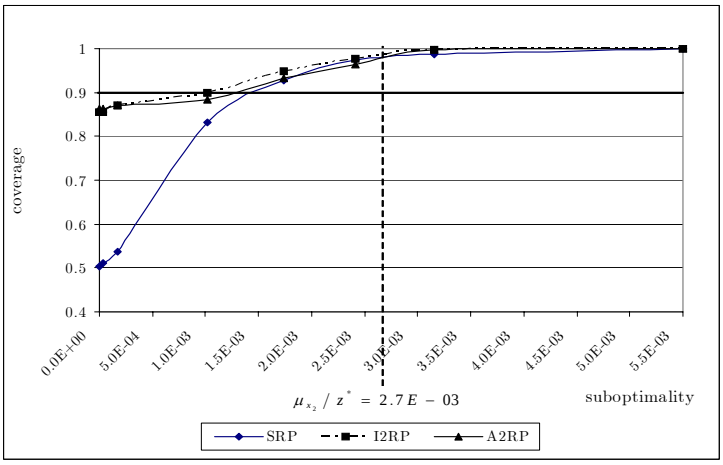

Figure 2.3: This figure is similar to Figure 2.2 except that $\hat{x} = x_2$.

Chapter 3

Assessing Solution Quality: Sequential Sampling Procedures

In the previous chapter, we examined several Monte Carlo sampling-based methods to form confidence intervals on the optimality gap. After carrying out such a procedure, we have a $(1-\alpha)$-level confidence interval on $\hat{x}$'s optimality gap. However, the sample size n is input to the procedure and it is possible that the width of the CI is so large that the result is of little practical value. An interval can be too wide due to one or more of the following three factors.

1. $\hat{x}$ is far from optimal,
2. The bias of z_n^* is large,
3. The sampling error is large.

The first factor depends on the quality of the candidate solution, $\hat{x}$. If $\hat{x}$ is found by solving an instance of $(SP_{n_{\hat{x}}})$ then consistency results, which establish conditions under which accumulation points of $\{x^*_{n_{\hat{x}}}\}$ solve (SP), imply that the contribution of factor 1 decreases as $n_{\hat{x}}$ grows (e.g., [19]). That said, in our subsequent development in this chapter we regard $\hat{x}$ as fixed and in the next chapter we explicitly consider allowing $n_{\hat{x}}$ to grow. The second

factor, bias, decreases as n grows and is asymptotically zero under mild conditions. The sampling error also decreases as n (and in case of MRP, n_g) grows. However, we do not know the sample size required to reduce these factors to a desired level. One way to reduce the sampling error is to employ variance reduction techniques [4, 16, 25, 33]. There is also work towards decreasing bias for some specially structured multi-stage stochastic problems [13].

In this chapter, in addition to assumptions (A1)-(A3) stated in Section 1.2, we assume

(A4) (SP) has a unique optimum solution, x^*.

We seek a priori control over the width of the confidence interval on the optimality gap. Suppose we want the width of this CI to be a prespecified value, say ϵ. With $\hat{x}$ fixed, the sampling error and the bias go to zero as $n \to \infty$. However, we cannot expect to shrink the CI width below the optimality gap of $\hat{x}$. Therefore, ϵ cannot be less than $\mu_{\hat{x}}$ and we can only control $h = \epsilon - \mu_{\hat{x}}$. Then, the asymptotically appropriate sample size required to reach a desired precision of h, from the perspective of controlling the sampling error is given by

$$n(h) = \inf_n \left\{ n \geq \frac{z_\alpha^2 \sigma_{\hat{x}}^2(x^*)}{h^2} \right\}, \tag{3.1}$$

where, as in Chapter 2, $\sigma_{\hat{x}}^2(x^*)$=var $[f(\hat{x}, \tilde{\xi}) - f(x^*, \tilde{\xi})]$. Bias is also a decreasing function of the sample size but the rate varies by problem class and this rate as well as the proportionality constant are not known in general. Therefore, (3.1) only partially controls the CI width. Since $\sigma_{\hat{x}}^2(x^*)$ is not known, (3.1)

cannot be calculated, so we estimate it with $s_n^2(x_n^*)$. Based on this simple idea, in this chapter we develop sequential sampling procedures for constructing a CI on the optimality gap.

Since in this chapter we develop sequential procedures for forming a confidence interval on the optimality gap, we begin by reviewing sequential methods for forming a confidence interval of the mean of a distribution or the mean performance measure of a general stochastic system and compare these with associated fixed-sample size procedure. We leave it to Chapter 4 to review sequential sampling methods for solving stochastic programs. In Section 3.2, we develop a fully sequential method where the sample size is increased one by one. Then, in Section 3.3 we extend this to an accelerated procedure, where the sample size is increased in jumps. In Section 3.4, we test the procedures for the newsvendor problem which was also used in Chapter 2 and in Section 4.5 we discuss computational effort. We end the chapter with concluding remarks.

3.1 Literature Review

Much of classical statistical theory deals with drawing inferences from data where the sample size, n, is fixed. In sequential estimation, the sample size is not fixed but depends on the observations collected so far and hence is a random variable. As a result, sequential estimation is closely related to the study of random walks hitting prespecified sets [24]. Sequential sampling methods were first developed by British and American statisticians during

World War II for hypothesis testing. Since then the use of sequential sampling has expanded in many directions and has been applied to problems in reliability, quality control and statistical clinical testing. For a variety of different applications and areas where sequential estimation is used, see [21], and for a more theoretical point of view, see [22].

It is not our intent to give a comprehensive review of sequential estimation. Instead, in the remainder of this section we focus on estimating a population mean. Here, we define sequential sampling procedures and contrast them with the traditional fixed-sample size procedure, emphasizing confidence interval construction. Sequential sampling procedures for estimating the mean are used in estimating the location parameter of a distribution (e.g., the mean of a normal distribution) or in estimating a complex stochastic system's mean performance measure (e.g., long-run average cycle time of a queueing network) through simulation. Before defining sequential sampling, let us first look at the standard fixed-sample size procedure and examine its properties.

Fixed-sample size procedure: To estimate the mean using a fixed-sample size procedure, a fixed number, n, of i.i.d. realizations $X^1, X^2, ..., X^n$ are sampled from a common distribution with mean μ and variance $\sigma^2 < \infty$. The sample mean $\bar{X}_n = \frac{1}{n}\sum_{i=1}^{n} X^i$ is calculated as an estimator of the mean. $\bar{X}_n$ is an unbiased estimator, $E[\bar{X}_n] = \mu$. It is also a strongly consistent estimator. That is, $\bar{X}_n \to \mu$ with probability one (w.p.1) as $n \to \infty$ by the strong law of large numbers (SLLN). The central limit theorem (CLT) establishes that the scaled errors converge to a normal random variable, $\sqrt{n}(\bar{X}_n - \mu) \Rightarrow N(0, \sigma^2)$.

There are also a number of other facts we can state from probability theory such as the law of iterated logarithms, large deviation results, etc. Using the CLT, for a given $0 < \alpha < 1$, it is possible to construct an approximate $(1-\alpha)$-level confidence interval (CI) for μ by

$$\left[\bar{X}_n \ - \ t_{n-1,\alpha/2}\sqrt{\frac{s_n^2}{n}} \ , \ \ \bar{X}_n \ + \ t_{n-1,\alpha/2}\sqrt{\frac{s_n^2}{n}} \right], \tag{3.2}$$

where $t_{n-1,\alpha/2}$ is the $1-\alpha/2$ quantile of the Student's t distribution with $n-1$ degrees of freedom and $s_n^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X^i - \bar{X}_n)^2$ is the sample variance. Note that in our setting of (SP), all of the above statements are valid for an i.i.d. sample of $\tilde{\xi}^1, \tilde{\xi}^2, ..., \tilde{\xi}^n$ from the distribution of $\tilde{\xi}$ yielding $f(x,\tilde{\xi}^1), ..., f(x,\tilde{\xi}^n)$ from the distribution of $f(x,\tilde{\xi})$ with sample mean $\bar{f}_n(x) = \frac{1}{n}\sum_{i=1}^{n} f(x,\tilde{\xi}^i)$ and population mean $E[f(x,\tilde{\xi})]$ for any fixed $x \in X$, provided $E[f^2(x,\tilde{\xi})] < \infty$.

The main disadvantage of the fixed-sample size procedure is that we cannot control the error associated with our estimate. When n is too small, the precision of the estimate can be low, depending on the variance of the underlying stochastic system. When n is too large, we use an unnecessarily large number of samples. This maybe undesirable if the cost of obtaining an observation is high. Suppose we would like to obtain a CI with a fixed half-width of h. Then, we cannot simply apply a fixed-sample size procedure to cover μ with the desired probability $1-\alpha$ since we do not know σ^2. If σ^2 were known, the number of observations needed to obtain such a CI is given by

$$n(h) = \inf_n \left\{ n \geq \frac{z_{\alpha/2}^2 \sigma^2}{h^2} \right\}, \tag{3.3}$$

where $z_{\alpha/2}$ is the $1-\alpha/2$ quantile of the standard normal distribution. If $n(h)$ is used as the fixed-sample size to construct confidence intervals for μ then the CI $\left[\bar{X}_{n(h)}-h,\, \bar{X}_{n(h)}+h\right]$ will have the desired coverage probability of $1-\alpha$. Of course, since σ^2 is not known, (3.3) cannot be calculated.

Two-stage procedure for normal samples: When the observations come from a normal distribution with unknown mean and variance, Stein [64, 65] showed that it is possible to obtain the desired coverage probability using a two-stage sampling procedure. In Stein's approach, an initial sample size of n_0 is used to estimate the variance by $s^2_{n_0}$. Then, the number of samples needed is estimated through

$$N_S(h) = \left\lceil z^2_{\alpha/2} s^2_{n_0}/h^2 \right\rceil,$$

where $\lceil\cdot\rceil$ returns the smallest integer greater than or equal to its argument. If n_0 is greater than this number, then the procedure stops. Otherwise, $N_S - n_0$ additional observations are drawn and the confidence interval $\left[\bar{X}_{N_S}-h,\, \bar{X}_{N_S}+h\right]$ is produced. For the two-stage procedure, $P(\mu \in \left[\bar{X}_{N_S}-h,\, \bar{X}_{N_S}+h\right]) \geq 1-\alpha$. This result holds for the normal distribution but is not true in general.

Sequential sampling procedure: Chow and Robbins [14] extended Stein's result to include non-normal distributions in a fully sequential setting. Their procedure adds one sample at a time and stops when $s^2_n + 1/n$ drops below $nh^2/z^2_{\alpha/2}$ (for continuous distributions, there is no need to inflate the sample variance by $1/n$). Let $N_{CR}(h)$ be the sample size when the procedure stops. For the Chow-Robbins procedure, $\lim_{h\to 0} P(\mu \in [\bar{X}_{N_{CR}(h)}-h,\, \bar{X}_{N_{CR}(h)}+h]) =$

$1-\alpha$, a property known as *asymptotic validity* (see Section 1.2). However, unlike Stein's procedure the actual coverage when the procedure terminates for a fixed $h > 0$ may be lower than the desired $1-\alpha$. Analogous properties hold for the fixed-sample size procedure of (3.2) when the underlying variables are non-normal. That is, the actual coverage of the CI in (3.2) may be lower than the desired level for a given n but as n grows large, the desired coverage is guaranteed by the CLT. Other asymptotic results of the Chow-Robbins procedure are $N_{CR}(h)/n(h) \to 1$, w.p.1 and $E[N_{CR}(h)]/n(h) \to 1$, as $h \to 0$, where $n(h)$ is given in (3.3). This last property is known as *asymptotic efficiency*.

Specifying a fixed-width of $2h$ in the above procedures yields a confidence interval with a desired *absolute precision*. An alternative is to specify a *relative-width* of γ such that $|\bar{X}_n - \mu|/|\mu| = \gamma$. Nadas [46] extended the Chow-Robbins procedure to handle a relative-width sequential confidence interval. There are various extensions and further generalizations of these procedures, see for instance [22, Chapters 6-8].

Sequential sampling in simulation: For simulation of stochastic systems, the simulation run length takes place of the sample size n. The run length can be fixed prior to simulation, resulting in a lack of control of the precision of the estimator. Alternatively, the run length can be determined with a sequential procedure. For steady-state simulations, Law and Kelton [40] and Law, Kelton and Koening [42] survey sequential methods used for constructing fixed-width and relative-width confidence intervals for the mean

of a stochastic system. These include Nadas' procedure and procedures rooted in the Chow-Robbins approach as well as others that deal with autocorrelation when independent samples cannot be generated. However, most of the procedures that belong to the latter group (when independent samples cannot be generated) are not backed up with asymptotic theory. In this case, Glynn and Whitt [23] show that asymptotic validity of sequential stopping rules for simulations can be achieved if the estimation process obeys a functional central limit theorem and if there is a strongly consistent estimator of the asymptotic variance of the estimator. Alternatively, it suffices for the variance estimator to satisfy a functional weak law of large numbers. More recent work in the area of simulation involves selection from a number of alternative systems using sequential sampling [36, 37].

Empirical results from the literature (e.g., [40]) suggest that care must be taken in implementing sequential procedures. In particular, when h or γ is relatively large, these procedures can result in inappropriate early termination and low coverage probabilities. The performance of sequential procedures improves when the sample size or the simulation run length grows larger (i.e., when h or γ is sufficiently small), as the asymptotic theory suggests. This may be undesirable due to computational constraints. Nevertheless, sequential methods remain popular because of the attractiveness of automatically obtaining a specified precision.

3.2 Fully Sequential Procedure

In Chapter 2, we developed single and two-replication procedures to assess solution quality in stochastic programs. Let us recall the single replication procedure (SRP). The output of this procedure, given in (2.5), is a confidence interval on the optimality gap that consists of a point estimate of the gap plus a sampling error term. If we wish to control the sampling error, the asymptotically appropriate sample size that guarantees a desired precision of h, is given by (3.1). The gap estimate term in (2.5) contains bias, which is also a decreasing function of the sample size but both the rate at which it shrinks to zero and the associated proportionality constant differ by problem class. Of course, by demanding a smaller precision h, we also decrease the bias in estimation. Since $\sigma^2_{\hat{x}}(x^*)$ is not known, (3.1) cannot be calculated, so we estimate it. For reasons that will become apparent shortly, we inflate the sampling variance that we use in our sequential procedures by $\frac{1}{n-1}$,

$$v_n^2(x_n^*) = \frac{1}{n-1}\sum_{i=1}^{n}\left[(f(\hat{x},\tilde{\xi}^i) - f(x_n^*,\tilde{\xi}^i)) - (\bar{f}_n(\hat{x}) - \bar{f}_n(x_n^*))\right]^2 + \frac{1}{n-1}. \quad (3.4)$$

This is similar in spirit to the Chow-Robbins procedure [14]. Below we present the fully sequential procedure (FSP).

FSP:

Input: Desired values for $h > 0$, $0 < \alpha < 1$, an initial sample size $n_0 \geq 2$, and a candidate solution $\hat{x} \in X$.

Output: $(1-\alpha)$-level confidence interval on $\mu_{\hat{x}}$.

1. Set $n = n_0$, and
   sample i.i.d. observations $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^n$ from the distribution of $\tilde{\xi}$.

2. Solve (SP_n) to obtain x_n^*.

3. Calculate $v_n^2(x_n^*)$ according to (3.4). If $v_n^2(x_n^*) \leq h^2 n / z_\alpha^2$, then goto 4.

   Else, sample an additional i.i.d. observation $\tilde{\xi}^{n+1}$, from the distribution of $\tilde{\xi}$, set $n = n + 1$ and goto 2.

4. Calculate $G_n(\hat{x}) = \frac{1}{n} \sum_{i=1}^{n} (f(\hat{x}, \tilde{\xi}^i) - f(x_n^*, \tilde{\xi}^i))$ and output one-sided CI on $\mu_{\hat{x}}$,

$$[0, G_n(\hat{x}) + h].$$

We recommend using an initial sample size $n_0 \geq 50$. The sample size when FSP terminates is

$$N(h) = \inf_n \left\{ n \geq \frac{z_\alpha^2 v_n^2(x_n^*)}{h^2} \right\}. \tag{3.5}$$

Our goal is to show that the confidence interval formed when FSP terminates is asymptotically valid as h shrinks to zero. In the construction of (2.5) for the fixed-sample size SRP, we were able to show the analogous result by invoking the CLT as $n \to \infty$ for $\bar{f}_n(\hat{x}) - \bar{f}_n(x^*)$, which is simply a sample mean of i.i.d. random variables. In the sequential procedure, $\bar{f}_n(\hat{x}) - \bar{f}_n(x^*)$ is replaced by $\bar{f}_{N(h)}(\hat{x}) - \bar{f}_{N(h)}(x^*)$. The sample size, $N(h)$, of this sample mean is now a random variable and the standard CLT for i.i.d. random variables does not apply. In order to obtain large sample sizes, we must have $N(h)$ grow as h shrinks. It is for this reason that we use the inflated variance $v_n^2(x_n^*) =$

$s_n^2(x_n^*)+\frac{1}{n-1}$. If we instead simply used $s_n^2(x_n^*)$, then the probability $N(h) \leq m$ is bounded below by $P(x_m^* = \hat{x})$, which of course can be positive. That said, $N(h) \to \infty$ as $h \downarrow 0$ w.p.1 is not enough. Sufficient conditions to ensure sample means of i.i.d. random variables with a random sample size satisfy the desired CLT is given in the following theorem.

Theorem 3.1 (Anscombe's Theorem). *Let $X^1, X^2, ..., X^n$ be a sequence of i.i.d. random variables with mean μ and variance $0 < \sigma^2 < \infty$. Let $\{N(h) : h > 0\}$ be a family of positive, integer-valued random variables and $\{n(h) : h > 0\}$ be a family of positive numbers tending to infinity as $h \downarrow 0$. Let $\bar{X}_n = \frac{1}{n}\sum_{i=1}^n X^i$ and let ν be a positive random variable. If*

$$\frac{N(h)}{n(h)} \xrightarrow{p} \nu \text{ as } h \downarrow 0,$$

then,

$$\frac{\bar{X}_{N(h)} - \mu}{\sigma/\sqrt{N(h)}} \Rightarrow N(0,1) \text{ as } h \downarrow 0,$$

where $\xrightarrow{p}$ denotes convergence in probability and $\Rightarrow$ denotes convergence in distribution.

Anscombe [2] first proved the above theorem with ν being a positive constant (degenerate positive random variable). Réyni [50] extended Anscombe's result to where ν is a positive discrete random variable. The theorem stated as above in its general form, where ν is a positive, not necessarily discrete, random variable is given in Blum et al. [11]. Before we show asymptotic validity of the fully sequential procedure, we need the following

lemma that establishes consistency of the sample variance estimator when the sample size is random.

Lemma 3.2. *Assume (A1)-(A4) and that* $\tilde{\xi}^1, \tilde{\xi}^2, \ldots$ *are i.i.d. as* $\tilde{\xi}$*. If* $N(h) \to \infty$*, w.p.1, as* $h \downarrow 0$*, then*

$$v^2_{N(h)}(x^*_{N(h)}) \to \sigma^2_{\hat{x}}(x^*), \quad \textit{w.p.1 as } h \downarrow 0.$$

Proof. Let ω denote a sequence of realizations of $\tilde{\xi}^1, \tilde{\xi}^2, \ldots$ and define $A = \{\omega : x^*_n(\omega) \nrightarrow x^* \text{ as } n \to \infty\}$, $B = \{\omega : v^2_n(x^*_n(\omega), \omega) \nrightarrow \sigma^2_{\hat{x}}(x^*) \text{ as } n \to \infty\}$, $C = \{\omega : N(h, \omega) \nrightarrow \infty \text{ as } h \downarrow 0\}$ and $D = \{\omega : v^2_{N(h,\omega)}(x^*_{N(h,\omega)}(\omega), \omega) \nrightarrow \sigma^2_{\hat{x}}(x^*) \text{ as } h \downarrow 0\}$. By assumption, as $h \downarrow 0$, $N(h) \to \infty$, w.p.1. This coupled with Proposition 2.1 and $D \subset (A \cup B \cup C)$ proves the assertion. □

Lemma 3.2 differs from part (iii) of Proposition 2.1 only in that the deterministic sequence of sample sizes in Proposition 2.1 is now replaced with a random sequence of sample sizes that also tend to infinity. Note that we assume unique optimality in this chapter, so, part (iii) of Proposition 2.1 simply states $\lim_{n\to\infty} s^2_n(x^*_n) = \sigma^2_{\hat{x}}(x^*)$, w.p.1 under this assumption. We are now ready to state the asymptotic validity result for the fully sequential method.

Theorem 3.3. *Assume (A1)-(A4) and that* $\tilde{\xi}^1, \tilde{\xi}^2, \ldots$ *are i.i.d. as* $\tilde{\xi}$*. Then for the FSP, if* $h > 0$*, then* $P(N(h) < \infty) = 1$ *and*

$$\lim_{h \downarrow 0} P(\mu_{\hat{x}} \leq G_{N(h)}(\hat{x}) + h) \geq 1 - \alpha. \tag{3.6}$$

Proof. Given $h > 0$, $P(N(h) = \infty) = \lim_{m\to\infty} P(N(h) > m)$

$$\leq \lim_{m\to\infty} P(m < z_\alpha^2 v_m^2(x_m^*)h^{-2}) = 0,$$

since $v_m^2(x_m^*) \to \sigma_{\hat{x}}^2(x^*) < \infty$, w.p.1 by Lemma 3.2. Thus, $P(N(h) < \infty) = 1$.

When $\hat{x} = x^*$ inequality (3.6) is trivial. Suppose $\hat{x} \neq x^*$. By the definition of $N(h)$,

$$\frac{z_\alpha^2 v_{N(h)}^2(x_{N(h)}^*)}{h^2} \leq N(h) \leq n_0 + \frac{z_\alpha^2 v_{N(h)-1}^2(x_{N(h)-1}^*)}{h^2}.$$

Dividing by $n(h) = \frac{z_\alpha^2 \sigma_{\hat{x}}^2(x^*)}{h^2}$ and taking limits as $h \downarrow 0$,

$$\frac{N(h)}{n(h)} \to 1, \quad \text{w.p.1}$$

by Lemma 3.2. This implies convergence in probability. Hence, using Anscombe's Theorem with $X^i = f(\hat{x}, \tilde{\xi}^i) - f(x^*, \tilde{\xi}^i)$ and following the same arguments as in the proof of Theorem 2.2, we obtain

$$\begin{aligned}
& \lim_{h\downarrow 0} P(\mu_{\hat{x}} \leq G_{N(h)}(\hat{x}) + h) \\
= & \lim_{h\downarrow 0} P\left(\frac{(\bar{f}_{N(h)}(\hat{x}) - z_{N(h)}^*) - \mu_{\hat{x}}}{v_{N(h)}(x_{N(h)}^*)/\sqrt{N(h)}} \geq -z_\alpha \right) \\
\geq & \lim_{h\downarrow 0} P\left(\frac{(\bar{f}_{N(h)}(\hat{x}) - \bar{f}_{N(h)}(x^*)) - \mu_{\hat{x}}}{\sigma_{\hat{x}}(x^*)/\sqrt{N(h)}} \geq -z_\alpha \frac{v_{N(h)}(x_{N(h)}^*)}{\sigma_{\hat{x}}(x^*)} \right) \\
= & 1 - \alpha
\end{aligned}$$

since as $h \downarrow 0$, $\frac{v_{N(h)}(x_{N(h)}^*)}{\sigma_{\hat{x}}(x^*)} \to 1$, w.p.1. □

By Theorem 3.3 we have established that the FSP yields an asymptotically valid CI on the optimality gap. In the limit, both SRP and FSP

behave in a similar way, that is, as $h \downarrow 0$, and as the sample size increases, both contain the optimality gap $\mu_{\hat{x}}$ with the desired probability, as given in (2.6) and (3.6), and also $\frac{N(h)}{n(h)} \to 1$, w.p.1. One drawback of using the FSP for stochastic programs is that the sample size is incremented one at a time and a new optimization problem is solved each time a new observation is added. In the next section, we extend FSP to increment the sample size by more than one observation.

3.3 Accelerated Sequential Procedure

Unlike many statistical problems where data naturally comes in a sequential fashion, in the problems we consider, it is easy to generate random observations of $\tilde{\xi}$. The computational bottleneck comes from solving a new optimization problem after a new scenario is added. Even when using warm-start techniques this is burdensome. One way to decrease the associated computational effort is to add more than one scenario at a time in Step 3 of the FSP. Although not as efficient as the FSP, in the sense that we might use more samples, this can accelerate solution times.

Below we state the accelerated sequential procedure (ASP), which uses the current estimate of $\sigma^2_{\hat{x}}(x^*)$ to increment the sample size. The procedure stops when the sample size estimate is less than or equal to the current sample size. Recall that $\lceil \cdot \rceil$ returns the smallest integer greater than or equal to its argument.

ASP:

Input: Desired precision value for $h > 0$, and $0 < \alpha < 1$, an initial sample size $n_0 \geq 2$, and a candidate solution $\hat{x} \in X$.

Output: $(1-\alpha)$-level confidence interval on $\mu_{\hat{x}}$.

1. Set $N_0(h) = n_0$ and sample $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^{N_0(h)}$ i.i.d. observations from the distribution of $\tilde{\xi}$. Set $t = 0$.

2. Solve $(\mathrm{SP}_{N_t(h)})$ to obtain $x^*_{N_t(h)}$

3. Calculate

$$N_{t+1}(h) = \max\left\{N_t(h), \quad \left\lceil \frac{z_\alpha^2 v^2_{N_t(h)}(x^*_{N_t(h)})}{h^2} \right\rceil \right\}, \tag{3.7}$$

where $v^2_{N_t(h)}(x^*_{N_t(h)})$ is defined as in (3.4).

If $N_{t+1}(h) = N_t(h)$ then set $T = t+1$ and goto 4.

Else, sample $N_{t+1}(h) - N_t(h)$ additional i.i.d. observations $\tilde{\xi}^{N_t(h)+1}$, $\tilde{\xi}^{N_t(h)+2}, ..., \tilde{\xi}^{N_{t+1}(h)}$, set $t = t+1$ and goto 2.

4. Calculate $G_{N_T(h)}(\hat{x}) = \frac{1}{N_T(h)} \sum_{i=1}^{N_T(h)} (f(\hat{x}, \tilde{\xi}^i) - f(x^*_n, \tilde{\xi}^i))$ and output one-sided CI on $\mu_{\hat{x}}$,

$$[0, G_{N_T(h)}(\hat{x}) + h].$$

For the ASP, instead of increasing the sample size one by one, we make larger, more intelligent increments by estimating the sample size needed using the current information so far. The procedure stops when the sample size

estimate is less than or equal to the current sample size. T denotes the number of iterations of the ASP, and it is a random variable. So, if the procedure stops with only solving one stochastic program and $N_1(h) = N_0(h)$ then $T = 1$, if the procedures stops when $N_2(h) = N_1(h)$ then $T = 2$ and so on. As before, we typically take an initial sample size $n_0 \geq 50$. $N_T(h)$ denotes the sample size when the procedure terminates. By construction, $N_T(h) \to \infty$, w.p.1 as $h \downarrow 0$. However, $N_T(h)$ is still a proper stopping time, that is, for a given $h > 0$, $P(N_T(h) < \infty) = 1$ and the ASP produces an asymptotically valid CI. This is summarized in the theorem below.

Theorem 3.4. *Assume (A1)-(A4) and that $\tilde{\xi}^1, \tilde{\xi}^2, \ldots$ are i.i.d. as $\tilde{\xi}$. Then for the ASP, if $h > 0$, then $P(N_T(h) < \infty) = 1$ and*

$$\lim_{h \downarrow 0} P(\mu_{\hat{x}} \leq G_{N_T(h)}(\hat{x}) + h) \geq 1 - \alpha. \tag{3.8}$$

Proof. Given $h > 0$,

$$\begin{aligned} P(N_T(h) = \infty) &= P\left(\bigcap_{k=1}^{\infty} \{N_k(h) > N_{k-1}(h)\}\right) \\ &= P\left(\bigcap_{k=1}^{\infty} \left\{ \left\lceil \frac{z_\alpha^2 v^2_{N_{k-1}(h)}(x^*_{N_{k-1}(h)})}{h^2} \right\rceil > N_{k-1}(h) \right\}\right). \end{aligned}$$

This has positive probability only if $v^2_{N_{k-1}(h)}(x^*_{N_{k-1}(h)}) \to \infty$ as $k \to \infty$, which is a contradiction.

When $\hat{x} = x^*$, inequality (3.8) is trivial. Suppose $\hat{x} \neq x^*$ and let $I_{\{\cdot\}}$ denote an indicator function. Then,

$$N_T(h) = n_0 I_{\{T=1\}} + \left\lceil \frac{z_\alpha^2 v^2_{n_0}(x^*_{n_0})}{h^2} \right\rceil I_{\{T=2\}} + \left\lceil \frac{z_\alpha^2 v^2_{N_{T-2}(h)}(x^*_{N_{T-2}(h)})}{h^2} \right\rceil I_{\{T \geq 3\}}.$$

Let $n(h) = \frac{z_\alpha^2 \sigma_{\hat{x}}^2(x^*)}{h^2}$ and let us examine each case in more detail. In the first case, since n_0 is fixed, there exists an h' such that for $\forall\ h \leq h'$, $P_h(T = 1) = 0$. In the second case, $N_T(h)/n(h) \xrightarrow{p} v_{n_0}^2(x_{n_0}^*)/\sigma_{\hat{x}}^2(x^*)$, a positive random variable. In the third case, if $P(v_{n_0}^2(x_{n_0}^*) \leq \sigma_{\hat{x}}^2(x^*))$ is positive, then, $N_T(h)/n(h) \xrightarrow{p} 1$, using (a conditional version) of Lemma 3.2. Combining these,

$$\frac{N_T(h)}{n(h)} \xrightarrow{p} \nu, \quad \text{as } h \downarrow 0,$$

where ν is a positive random variable that takes on value 1, with $P(v_{n_0}^2(x_{n_0}^*) \leq \sigma_{\hat{x}}^2(x^*))$ and $\nu = v_{n_0}^2(x_{n_0}^*)/\sigma_{\hat{x}}^2(x^*)$ otherwise. Hence, we can use Anscombe's theorem (Theorem 3.1). The rest of the proof is analogous to that of Theorem 3.3. □

From Theorem 3.4, we infer that for sufficiently small h, the confidence interval $[0, G_{N_T(h)}(\hat{x}) + h]$ formed using the ASP contains the optimality gap of $\hat{x}$, $\mu_{\hat{x}}$, with the desired probability $1 - \alpha$. So far, we have extended the single replication procedure of the previous chapter to a sequential confidence interval that controls the sampling error. We developed two methods, where we either increase the sample size one by one, or, in jumps of random size. In the development of these procedures, we assumed that (SP) has a unique optimum solution. Even though we do not develop the associated material explicitly here, extensions of our sequential SRPs to two-replication procedures are possible. In the next section, we compare the two sequential methods FSP and ASP empirically and discuss computational effort.

3.4 Empirical Coverage Results

Theorems 3.3 and 3.4 show that the confidence intervals formed by both the fully and accelerated sequential methods contain the optimality gap with a desired probability as $h \downarrow 0$. In this section, we examine their small-sample behavior by applying them to a newsvendor problem with uniform demand, which we also used in Chapter 2. We again use the candidate solution $\hat{x} = 8.775$ with $\mu_{\hat{x}} = 3\frac{1}{3}$, and $\sigma^2_{\hat{x}}(x^*) = 140.79$. For more details on the test problem, please refer to Section 2.4.1.

For our tests, we set $n_0 = 50$ and again take $\alpha = 0.10$. We look at four different values of h by decreasing its value by half each time. For each value of h, we repeat the procedures 1,000 times using independent streams. As before, we report coverage probabilities, $\hat{p}$, see Section 1.2. Table 3.1 lists coverage results for the fully and accelerated sequential procedures. Both procedures have good coverage for $h = 2$, which is close to the optimality gap, $\mu_{\hat{x}} = 3\frac{1}{3}$. Coverage of ASP seems to be better than FSP for smaller values of h.

	$\hat{p}$	
h	FSP	ASP
2	0.942 ± 0.012	0.939 ± 0.012
1	0.834 ± 0.019	0.873 ± 0.017
0.5	0.877 ± 0.017	0.896 ± 0.016
0.25	0.897 ± 0.016	0.916 ± 0.014

Table 3.1: Empiricial coverage results for FSP and ASP.

To see how the sequential procedures perform as $h \downarrow 0$, we compare coverage probabilities for a range of values of h. Figure 3.1 shows how the

h	$n(h)$	$N(h)$	$N_T(h)$
2	58	62.396 ± 0.983	71.332 ± 1.477
1	232	213.075 ± 3.760	285.918 ± 6.023
0.5	926	909.374 ± 7.505	1165.11 ± 21.441
0.25	3703	3680.50 ± 15.478	4700.93 ± 85.701

Table 3.2: Asymptotically correct sample sizes, $n(h)$, vs. sample sizes used by the FSP, $N(h)$, and the ASP, $N_T(h)$.

coverage changes as h shrinks to 0 for the two procedures. For any $h \geq \mu_{\hat{x}}$ we have 100% coverage because the CI is guaranteed to contain the optimality gap. When h is decreased from this value, coverage naturally decreases. As $h \downarrow 0$, coverage first drops and then starts to rise again. Note that $h = 2$ is 60% of the optimality gap $\mu_{\hat{x}} = 3.333$, and Figure 3.1 shows that the CI formed by $[0, G_{N(h)}(\hat{x}) + h]$ has a higher chance of covering the optimality gap compared to a smaller value of h. However, as $h \downarrow 0$, the asymptotic result appears to take hold; the coverage increases and is close to 90%. The results for the FSP and ASP are fairly similar for $h \geq 1.75$ (this corresponds to $h/\mu_{\hat{x}} \geq 52.5\%$) but the FSP has lower coverage for smaller values of h and its coverage seems to follow a more regular pattern.

In Table 3.2, we list the asymptotically correct sample sizes, $n(h)$, calculated using the population variance and the average sample size used by the procedures, $N(h)$ and $N_T(h)$, along with a 90% CI half-width for the expected sample size, for different values of h. For instance, a precision of $h = 1$ requires approximately 230 sample observations, and FSP on average used 213 and ASP used 285. As expected, the sample size grows approximately four

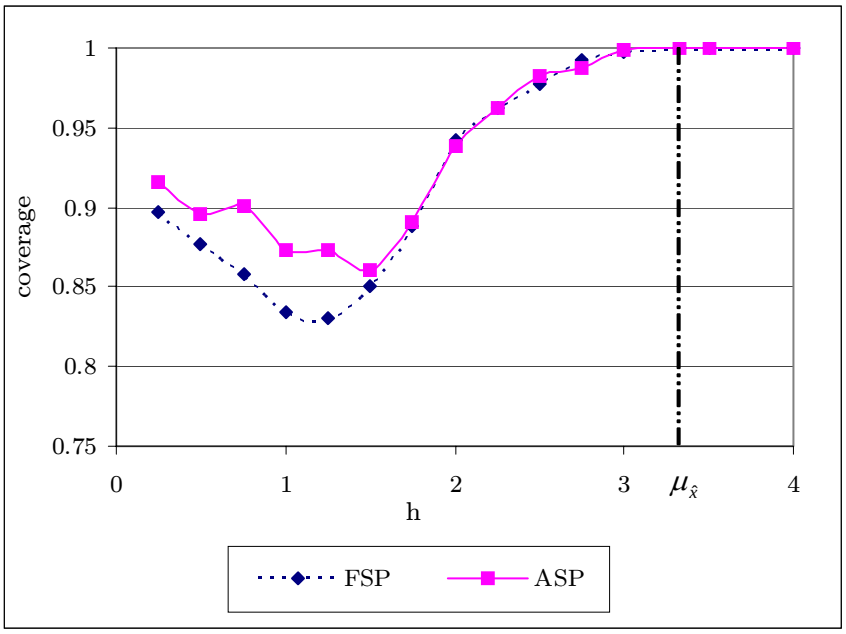

Figure 3.1: Comparison of sequential procedures: Coverage vs. h ($\alpha = 0.10$).

times when h is decreased by half. The FSP, on average, uses a sample size smaller than that specified by $n(h)$ and also has lower coverage compared to ASP. ASP, on the other hand, uses more samples than FSP and also more than that specified by $n(h)$.

We also examined the number of jumps made by ASP when applied to this instance of the newsvendor problem. In Table 3.3, we report the average number of iterations of the ASP, T, as defined in the procedure. Recall that T gives the total of number of stochastic programs solved by the ASP. For the problem we consider, on average, this number is less than 4.

h	T
2	1.886 ± 0.054
1	2.781 ± 0.064
0.5	3.086 ± 0.071
0.25	3.039 ± 0.069

Table 3.3: Average number of iterations for ASP.

3.5 Computational Effort

In this section, we discuss the computational effort required by the procedures of this and the previous chapter. Table 3.4 provides a summary of results for the different procedures applied to the newsvendor problem described in Section 2.4.1. We report n, the sample size for the fixed-sample procedures and $\bar{N}(h)$, the average sample size out of 1,000 replications used by the sequential procedures. This time, we also report the point estimate of the optimality gap and the resulting CI width on the optimality gap, along with a 90% confidence interval half-width on their expected values. Since newsvendor problem is essentially a quantile estimation problem, we coded it in C++ and used "quicksort" algorithm to find the optimum solution. The solution times reported in Table 3.4 are in seconds and they are the *total* solution time that 1,000 replications took for each procedure and for each sample size, or, for each value of h.

FSP is very slow because of re-optimization at each step. Even though ASP uses larger sample sizes, it is much faster and it also has better coverage. We recommend ASP over FSP. Both of these procedures are computationally expensive compared to fixed-sample size procedures, discussed in Chapter 2.

However, sequential methods may be preferred when the sampling error is large compared to the gap estimate. The two replication procedures have shorter solution times than SRP because solving two problems each with a sample size of $n/2$ is faster than solving one problem with a sample size of n.

3.6 Concluding Remarks

In this chapter, we have developed sequential sampling methods for assessing solution quality that control the sampling error. Unlike the fixed-sample size procedures developed in Chapter 2, the sample size for the sequential procedures depends on the data observed so far. For instance, in (3.7) for the accelerated procedure, we give a rule to increase the sample size using the current information obtained so far. Since the sample size is now a random variable, the analysis of sequential methods is somewhat different than their fixed-sample counterparts. For example, we have inflated the sampling variance by a factor of $\frac{1}{n-1}$, which leads to a slightly tighter stopping rule, given in (3.5).

The sequential methods presented in this chapter are computationally more expensive compared to the SRP, however, they do provide partial control over the width of the interval and serve to extend the results of Chow and Robbins [14] for sequential CI construction for the mean to testing solution quality for stochastic programs.

A final remark is that all of the procedures developed so far for assessing solution quality can be used within or after a separate algorithm that generates

Method	$n/\bar{N}(h)$	$\hat{p}$	Gap	CI	Sol Time
MRP	50	0.981 ± 0.007	3.662 ± 0.017	4.060 ± 0.018	1.171
($n_g = 30$)	100	0.973 ± 0.008	3.499 ± 0.011	3.777 ± 0.012	2.703
	500	0.943 ± 0.012	3.367 ± 0.005	3.490 ± 0.005	16.859
	1000	0.912 ± 0.015	3.346 ± 0.004	3.433 ± 0.004	36.718
SRP	50	0.872 ± 0.017	3.596 ± 0.087	5.703 ± 0.110	0.078
	100	0.880 ± 0.017	3.456 ± 0.062	4.986 ± 0.073	0.156
	500	0.892 ± 0.016	3.376 ± 0.028	4.056 ± 0.030	0.812
	1000	0.896 ± 0.016	3.358 ± 0.020	3.840 ± 0.021	1.687
I2RP	50	0.936 ± 0.013	3.830 ± 0.122	7.013 ± 0.140	0.046
	100	0.929 ± 0.013	3.596 ± 0.087	5.710 ± 0.092	0.141
	500	0.914 ± 0.014	3.402 ± 0.039	4.364 ± 0.039	0.718
	1000	0.912 ± 0.015	3.376 ± 0.028	4.056 ± 0.028	1.609
A2RP	50	0.915 ± 0.014	3.913 ± 0.087	6.138 ± 0.110	0.046
	100	0.902 ± 0.015	3.624 ± 0.061	5.117 ± 0.073	0.141
	500	0.908 ± 0.015	3.388 ± 0.027	4.070 ± 0.029	0.718
	1000	0.903 ± 0.015	3.369 ± 0.019	3.850 ± 0.020	1.609
FSP	62.40	0.942 ± 0.012	3.255 ± 0.089	5.255 ± 0.089	0.594
	213.01	0.834 ± 0.019	3.158 ± 0.056	4.158 ± 0.056	11.281
	909.37	0.877 ± 0.017	3.294 ± 0.027	3.794 ± 0.027	193.718
	3680.50	0.897 ± 0.016	3.318 ± 0.013	3.568 ± 0.013	3095.200
ASP	71.33	0.939 ± 0.012	3.261 ± 0.068	5.261 ± 0.068	0.219
	285.92	0.873 ± 0.017	3.212 ± 0.043	4.212 ± 0.043	1.140
	1165.11	0.896 ± 0.016	3.322 ± 0.020	3.822 ± 0.020	5.640
	4700.93	0.916 ± 0.014	3.325 ± 0.009	3.575 ± 0.009	25.953

Table 3.4: Comparison of various methods for assessing solution quality for the newsvendor problem.

candidate solutions. For example, such an algorithm can generate a candidate solution and this solution can be tested to see if it is near-optimal, either sequentially or with a fixed sample size. If the resulting CI width is large, then a new candidate solution needs to be generated. This scheme can terminate when the CI drops below a certain level. However, carrying out this idea naively can lead to poor coverage results, especially if it is repeated many times. So, in the next chapter, we develop a rigorous procedure along these lines that allows us to consider a sequence of candidate solutions.

Chapter 4

A Sequential Sampling Procedure for Solving Stochastic Programs

In this chapter, we present a Monte Carlo sampling-based procedure for solving stochastic programs by sequentially increasing the sample size. As we have mentioned before, many practical problems modeled as stochastic programs have a prohibitively large number of scenarios that prevents finding an exact solution in a reasonable amount of time. Monte Carlo sampling-based methods provide a means of approximation by replacing the expectations or probabilities that appear in stochastic programs by their sampling estimates. These methods are usually justified asymptotically, by providing conditions under which the approximating solutions solve (SP) as the sample size $n \to \infty$. However, practical implementations require a reliable means to terminate the procedure. In particular, such methods require a criteria for terminating that determines when the candidate solution's objective function value is sufficiently close to z^*, and rules to increase the sample size. Moreover, some statement regarding the quality of the solution obtained needs to be made.

In the previous chapters, we have developed several methods to determine if a candidate solution's objective function value is sufficiently close

to z^*. In this chapter, using these results we develop a sequential sampling procedure. In the procedure we propose, we assume that a sequence of candidate solutions with limit points that solve (SP) is given. One method to generate such a sequence is to solve a series of sampling problems with increasing sample size. However, we allow candidate solutions to be generated by any method. Given a candidate solution, we then assess its quality, using single or two-replication procedures developed in Chapter 2. We terminate the procedure when the optimality gap estimate of the current candidate solution falls below a certain level, depending on the variance estimate. We show that asymptotically this procedure finds a solution with a small optimality gap (of desired length) with a high (desired) probability.

In the remainder of the chapter, we first provide a literature review of sampling methods to solve problems of kind (SP), focusing on sequential methods. In Section 4.2, we state our sequential procedure and in Section 4.3 we prove desired theoretical properties. We then discuss implementation details and test the performance our procedure using problems from the literature. Finally, we end the chapter with concluding remarks.

4.1 Literature Review

As mentioned before, (SP) represents a large class of problems found in statistics and operations research. In statistics, a generalization of maximum likelihood estimators, called M-estimators [32], are another example that are of this form. M-estimators are solutions x_n^* to (SP_n), estimating a parameter

of interest x^* that solves (SP), and they include maximum likelihood and least squares estimators as special cases [34]. Sequential sampling procedures have been developed for M-estimators; see [31] and references cited therein. In these procedures, f is assumed to be differentiable in x and (SP_n) is equivalently defined by a (set of) equation(s) involving $\psi(x, \tilde{\xi}) = \nabla_x f(x, \tilde{\xi})$, called the score function and the focus is on estimation of x^*. In the optimization problems we consider, f is usually not differentiable and we are indifferent to how close we are to the set of optimum solutions as long as the objective function value is close to z^*.

For stochastic programming problems, there is relatively little work on sequential issues. In two-stage stochastic linear programs with recourse, for example, $f(\cdot, \tilde{\xi})$ is piecewise linear and convex and $E[f(\cdot, \tilde{\xi})]$ is convex and typically also non-smooth. *Stochastic quasigradient algorithms* can be applied in such cases; they mimic steepest descent in which gradients or subgradients of $E[f(x, \tilde{\xi})]$ are replaced by their sampling estimates. Ermoliev [20] surveys such methods and Pflug [49] surveys step size and stopping rules for stochastic quasigradient algorithms. One advantage of the stochastic quasigradient methods is that they are able to handle decision-dependent stochasticity. However, when used for solving two-stage stochastic linear programs with recourse (SLP-2), they do not make use of the special structure of these problems.

A method that works well for SLP-2 with discrete, finite number of scenarios is the so-called L-shaped method (also known as Benders' decomposition). Dantzig and Glynn [16] and Infanger [33] use sampling within the

L-shaped method. They change the sampling distribution, using a method called importance sampling, to reduce the variance in estimation. Dantzig and Infanger [17] and Periera and Pinto [48] use similar ideas for multi-stage models. Higle and Sen [29] use an L-shaped method with stochastic cuts. The cuts come from a single stream of observations and they are washed out in a manner guaranteed to ensure desirable asymptotics as the algorithm proceeds. For stochastic global optimization, Norkin, Pflug and Ruszczyński [47] use sampling within a branch-and-bound algorithm. Even though there is work with respect to when to stop the procedures, and how to assess the quality of the solutions resulting from these sampling-based methods [18, 26, 28], sequential issues that arise have not been addressed fully.

Instead of using sampling within an optimization algorithm such as L-shaped or branch-and-bound, other methods simply solve a series of sampling problems, (SP_n). Kleywegt et al. [63] analyze such a method for stochastic discrete optimization and Shapiro and Homem de Mello [60] do so for two-stage stochastic linear programs with recourse. Resampling is an essential part of selecting candidate solutions or assessing their quality in these methods. One feature of our sequential procedure is that a single stream of observations can be used, with increasing sample sizes, and resampling is not needed.

For stopping rules and rules to choose sample sizes regarding sampling-based methods to solve (SP), Morton [45] develops stopping rules theory for a class of algorithms that estimate a sequence of sampling-based upper and lower bounds on the optimal value by assuming the difference between upper and

lower bounds are normally distributed or satisfy (history-dependent) central limit theorems. For our procedure, we use the framework provided in this work. For convex, piecewise linear stochastic programs Shapiro, Homem de Mello and Kim [62] estimate the sample size needed to find the optimal solution with a given probability by estimating a so-called condition number.

4.2 Sequential Sampling Procedure

The procedure we propose is quite simple, and it involves solving a series of stochastic programs with sampled observations, (SP_{n_k}), with increasing sample sizes n_k at iteration k. Suppose at each iteration k, a feasible candidate solution $\hat{x}_k$ is given. We assume that the sequence of candidate solutions $\{\hat{x}_k\}$ has limit points in X^*, w.p.1. For instance, when $\hat{x}_k$ is generated by solving a sampling problem (SP_{m_k}) with sample size $m_k \to \infty$ as $k \to \infty$, then Proposition 2.1 states that under (A1)-(A3) and provided that $\tilde{\xi}^1, \ldots, \tilde{\xi}^{m_k}$ are i.i.d. as $\tilde{\xi}$, this asymptotic consistency condition is satisfied. That said, we allow $\{\hat{x}_k\}$ to be generated by any other method. In Chapters 2 and 3, the candidate solution $\hat{x}$ was input to the procedures. Similarly, in this chapter, the *sequence* of candidate solutions is an input to the sequential procedure. In saying that a method for generating $\hat{x}_k$ is an input to the procedure, we implicitly assume that the method to generate $\hat{x}_k$ does not depend on the observations used in the evaluation procedures.

Given a candidate solution $\hat{x}_k$ at iteration k, we check to see if it is a high quality solution. Recall that we define quality by the optimality gap,

$\mu_{\hat{x}_k} = E[f(\hat{x}_k, \tilde{\xi})] - z^*$ and a high quality solution as one with small optimality gap. Using a sample size of n, we estimate this quantity by:

$$G_n(\hat{x}_k) = \frac{1}{n}\sum_{i=1}^{n} f(\hat{x}_k, \tilde{\xi}^i) - \min_{x \in X} \frac{1}{n}\sum_{i=1}^{n} f(x, \tilde{\xi}^i), \tag{4.1}$$

where we use a common stream of random numbers, $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^n$, to calculate both terms in (4.1). Note that $G_n(\hat{x}_k) \geq 0$, w.p.1. Recall that for $x \in X$, we define $s_n^2(x) = \frac{1}{n-1}\sum_{i=1}^{n}[(f(\hat{x}_k, \tilde{\xi}^i) - f(x, \tilde{\xi}^i)) - (\bar{f}_n(\hat{x}_k) - \bar{f}_n(x))]^2$. Using the single replication procedure (SRP) presented in Section 2.2, we form a one-sided confidence interval on the optimality gap of the candidate solution $(\mu_{\hat{x}_k})$ by

$$\left[0,\ G_n(\hat{x}_k) + \frac{z_\alpha s_n(x_n^*)}{\sqrt{n}}\right]. \tag{4.2}$$

Under assumptions (A1)-(A3) and that $\tilde{\xi}^1, \tilde{\xi}^1, \ldots$ are i.i.d. as $\tilde{\xi}$, we have established in Theorem 2.2 that the CI given in (4.2) covers the optimality gap of $\hat{x}_k$ with desired probability, $(1-\alpha)$, when n is large enough. In our sequential procedure, at each iteration k, we assess the quality of the candidate solution $\hat{x}_k$ using $G_n(\hat{x}_k)$ and $s_n(x_n^*)$ with a sample size of $n = n_k$. For ease of notation, from now on we drop $\hat{x}_k$ and simply use $\mu_k = \mu_{\hat{x}_k} = E[f(\hat{x}_k, \tilde{\xi})] - z^*$, $G_k = G_{n_k}(\hat{x}_k)$ and $s_k = s_{n_k}(x_{n_k}^*)$.

At iteration k, we select a sample size, n_k, and generate i.i.d. observations $\tilde{\xi}^{n_{k-1}+1}, \ldots, \tilde{\xi}^{n_k}$ (we let $n_0 = 1$). Using the observations generated so far, we solve a sampling problem to assess the quality of this solution. If this solution satisfies a stopping criterion, we exit the procedure. If not, we select another sample size, $n_{k+1} \geq n_k$, generate additional observations

$\tilde{\xi}^{n_k+1}, \tilde{\xi}^{n_k+2}, \ldots, \tilde{\xi}^{n_{k+1}}$, and solve the resulting sampling problem to assess the quality of the new candidate solution $\hat{x}_{k+1}$. We stop at iteration T when the following stopping criterion is satisfied,

$$T = \inf_{k \geq 1} \{G_k \leq h s_k + \epsilon'\}. \tag{4.3}$$

The random stopping time T is the first time G_k's width relative to s_k falls below h plus a small nonnegative number ϵ', which ensures finite stopping (see next section). We can add the condition $\{s_k \leq b\}$ to (4.3) so that when we stop G_k is below a certain threshold, $hb + \epsilon'$.

When we stop, we would like to make probabilistic statements about the candidate solution at the stopping iteration. For instance, we would like this candidate solution to be of high quality (near optimal) with a desired probability. For the procedure we propose, below we show that for $\epsilon > h$,

$$\liminf_{\epsilon \downarrow h} P\left(\mu_T \leq \epsilon s_T + a_T + \epsilon'\right) \geq 1 - \alpha. \tag{4.4}$$

In other words, the optimality gap of $\hat{x}_T$, the candidate solution when we stop, is a small fraction of the sampling variance plus an inflation factor of a_T and ϵ', with a desired probability for ϵ close enough to h. As before, if we have the additional condition $\{s_T \leq b\}$, then, we asymptotically guarantee that the optimality gap of $\hat{x}_T$ to be at most $\epsilon b + \epsilon'$ plus an inflation factor of a_T, with a confidence level of $1 - \alpha$. This inflation factor, a_k, can be any positive sequence of numbers such that $a_k \downarrow 0$ as $k \to 0$. Examples include $a_k = 1/k$, or, $1/\sqrt{k}$. Inflating the confidence region (as we did in (4.4) by adding a_k), or

alternatively, tightening the stopping criterion (as we did in (3.5) by inflating the variance) is fairly standard when using sampling methods with a sequential nature [14, 23].

At iteration k, we choose the sample size according to

$$n_k \geq \left(\frac{1}{\epsilon - h}\right)^2 \left(c_p + 2pa_k^{-2} \ln^2 k\right), \tag{4.5}$$

where $c_p = \max\{2 \ln \left(\sum_{k=1}^{\infty} k^{-p\, a_k^{-2} \ln k} / \sqrt{2\pi}\alpha\right), 1\}$. Here, $p > 0$ is a parameter that affects the number of samples we generate during the procedure. We discuss how to choose p in more detail below. The sample size growth formula for the sequential procedure given in (4.5) is proportional to $(\epsilon - h)^{-2}$, it has a constant term, c_p, which depends on p, and it grows of order $O(a_k^{-2} \ln^2 k)$ with respect to the iteration number k. For example, when a_k is chosen to be $1/\sqrt{k}$, the sample size grows of $O(k \ln^2 k)$ and when $a_k = 1/k$, it grows of $O(k^2 \ln^2 k)$. Thus, the faster the a_k tends to 0, guaranteeing a smaller optimality gap of the stopping candidate solution through (4.4), the larger the sample sizes, n_k, we need. Note that the sample size growth is bounded below by $O(\ln^2 k)$.

In the next section, we show when the sample size is chosen to satisfy (4.5) then, (4.4) holds under a finite moment generating function assumption. We also show the procedure stops in a finite number of steps.

4.3 Asymptotic Validity and Finite Stopping

For the sequential sampling method presented above, the stopping time as well as the solution provided by the algorithm are both random variables.

Therefore, statements regarding finite stopping and the quality of the solution provided by the algorithm need to be stated in a probabilistic fashion. In this section, we first present a result that shows (4.4) holds for the sequential procedure described above, under a finite moment generating function assumption. Then, we prove and discuss the finite stopping of the algorithm. We also provide a generalization where we relax the moment generating function assumption and replace it with a finite r^{th} moment assumption.

4.3.1 Finite Moment Generating Function

Recall that for $x \in X$, we use the notation, $\bar{f}_n(x) = \frac{1}{n}\sum_{i=1}^{n} f(x, \tilde{\xi}^i)$. and given a candidate solution $\hat{x} \in X$, we let $\sigma^2_{\hat{x}}(x) = \text{var}[f(\hat{x}, \tilde{\xi}) - f(x, \tilde{\xi})]$. Also, recall that X^* denotes the set of optimum solutions. In the previous chapters, we fixed the candidate solution, $\hat{x}$, and used variances such as $\sigma^2_{\hat{x}}(x^*_{\text{min}})$, where $x^*_{\text{min}} \in \arg\min_{x \in X^*} \text{var}[f(\hat{x}, \tilde{\xi}) - f(x, \tilde{\xi})]$. Note that the definition of x^*_{min} depends on the candidate solution $\hat{x}$, and it is the optimal solution to (SP) with the minimum variance of $f(\hat{x}, \tilde{\xi}) - f(x, \tilde{\xi})$. In this chapter, we allow $\hat{x}$ to change and for ease of exposition, simply denote $\sigma^2_{\hat{x}}(x^*_{\text{min}})$ as $\sigma^2(\hat{x})$.

For any $x \in X$, due to the minimization of the sample mean, we have the following inequality

$$G_n(x) = \bar{f}_n(x) - \bar{f}_n(x^*_n) \;\geq\; \bar{f}_n(x) - \bar{f}_n(x^*_{\text{min}}) = D_n(x), \tag{4.6}$$

where x^*_{min} is defined for this x. When $0 < \sigma^2(x) < \infty$, we have

$$\sqrt{n}(D_n(x) - \mu_x) \Longrightarrow N(0, \sigma^2(x)) \quad \text{as } n \to \infty. \tag{4.7}$$

With x and hence $x^*_{\min}$ fixed, $D_n(x)$ is a sample mean of i.i.d. random variables, therefore, (4.7) follows directly from the central limit theorem. If $\sigma^2(x) = 0$, then, $f(x,\tilde{\xi}) - f(x^*,\tilde{\xi}) = c$, for almost all $\tilde{\xi}$, where c is a constant. We are interested in the moment generating function (MGF) of the variables $D_n(x)$. When $\sigma^2(x) = 0$, $D_n(x)$ is constant for all n and therefore has an MGF. When $\sigma^2(x) > 0$, we assume that the MGF of the scaled random variables $\sqrt{n}(D_n(x) - \mu_x)/\sigma(x)$ exists, i.e.,

$$\sup_{x\in X} E\left[e^{\gamma\left(\frac{D_n(x)-\mu_x}{\sigma(x)/\sqrt{n}}\right)}\right] < \infty \text{ for } |\gamma| \leq \gamma_0. \tag{4.8}$$

This assumption can be somewhat restrictive, however, it is satisfied when X is compact (our assumption (A3)) and the distribution of $\tilde{\xi}$ has bounded support. More generally, with X compact, the MGF exists when (SP) satisfies the following Lipschitz condition with the Lipschitz constant $K(\tilde{\xi})$, for almost all $\tilde{\xi}$, such that

$$|f(x_1,\tilde{\xi}) - f(x_2,\tilde{\xi})| \leq K(\tilde{\xi})\|x_1 - x_2\|, \tag{4.9}$$

for $\forall\, x_1, x_2 \in X$ and $E[e^{\gamma K(\tilde{\xi})}] < \infty$ for some $|\gamma| \leq \gamma_0$. Recall that for two-stage stochastic linear programs with fixed recourse,

$$\begin{aligned} f(x,\tilde{\xi}) = cx \;+\; & \min_{y\geq 0} \quad \tilde{q}y \\ & \text{s.t} \quad Wy = \tilde{r} - \tilde{T}x. \end{aligned}$$

Suppose $(\tilde{q},\tilde{r},\tilde{T})$ can be expressed as a linear combination of $\tilde{\xi}$ with independent components. Note that this allows for first-order dependencies between

the components of $(\tilde{q}, \tilde{r}, \tilde{T})$. Then, the Lipschitz condition (4.9) and hence the MGF assumption (4.8) will be satisfied when the squared Euclidean norm of the random vector, $\tilde{\xi}$ has an MGF, i.e. $E[e^{\gamma\|\tilde{\xi}\|^2}] < \infty$ for some $|\gamma| \leq \gamma_0$; see e.g., [51].

Below we state and prove the validity of the sequential sampling procedure under the existence of the moment generating function. Our result, given in (4.4), is asymptotic, as $\epsilon \downarrow h$, i.e., as the sample sizes grow. We note that even in the simple case of constructing confidence intervals for the mean by sequential sampling, the validity of the resulting confidence intervals (i.e., that the confidence interval has the desired coverage probability) is proven asymptotically, e.g., [14]. To prove (4.4) holds, we make use of Fatou's Lemma, which provides conditions and the direction of inequality when "lim inf" or "lim sup" and an integral (or, an infinite sum) are exchanged.

Lemma 4.1 (Fatou's Lemma). *(i) Suppose $\{f_n\}$ is a sequence of non-negative measurable functions in a measure space E, then,*

$$\int_E \liminf_{n\to\infty} f_n \leq \liminf_{n\to\infty} \int_E f_n.$$

(ii) If in addition, $L \leq f_n \leq U$ for all n, such that $\int_E L < \infty$ and $\int_E U < \infty$, then,

$$\int_E \liminf_{n\to\infty} f_n \leq \liminf_{n\to\infty} \int_E f_n \leq \limsup_{n\to\infty} \int_E f_n \leq \int_E \limsup_{n\to\infty} f_n.$$

Proof. For proof of part (i), see e.g., [54]. Part (ii) follows from applying part (i) to $(f_n - L)$ and $(U - f_n)$, both non-negative, and by

$$\liminf_{n\to\infty} (f_n - L) = \liminf_{n\to\infty} f_n - L \quad \text{and} \quad \liminf_{n\to\infty} (U - f_n) = U - \limsup_{n\to\infty} f_n.$$

□

Before we present the theorem, we recall the following bound on the tails of a standard normal [12, p.185].

Lemma 4.2 (Bound on tail of a standard normal). *Let Z be a standard normal, then,*

$$P(Z \geq t) \leq \frac{1}{\sqrt{2\pi}} \frac{e^{-t^2/2}}{t}.$$

Theorem 4.3. *Assume (A1)-(A3) and that $\tilde{\xi}^1, \tilde{\xi}^2, \ldots$ are i.i.d. as $\tilde{\xi}$, and assume (4.8) holds. Let $M^2 = \max_{x\in X} \sigma^2(x)$ and take $p > (\epsilon - h)^2 M^2 / 2\gamma_0^2$ and $0 < \alpha < 1$. Then, for the sequential sampling procedure where the sample size is increased according to (4.5), and the procedure stops at iteration T according to (4.3),*

$$\liminf_{\epsilon \downarrow h} P\left(\mu_T \leq \epsilon s_T + a_T + \epsilon'\right) \geq 1 - \alpha.$$

Proof. When we stop, $G_T \leq hs_T + \epsilon'$ implies,

$$\begin{aligned} P\left(\mu_T \geq \epsilon s_T + a_T + \epsilon'\right) &\leq P\left(\mu_T \geq G_T - hs_T + \epsilon s_T + a_T\right) \\ &= \sum_{k=1}^{\infty} P\left(G_1 > hs_1 + \epsilon', \ldots, G_k \leq \mu_k - (\epsilon - h)s_k - a_k\right) \\ &\leq \sum_{k=1}^{\infty} P\left(G_k - \mu_k \leq -(\epsilon - h)s_k - a_k\right) \\ &\leq \sum_{k=1}^{\infty} P\left(D_k - \mu_k \leq -(\epsilon - h)s_k - a_k\right) \qquad (4.10) \end{aligned}$$

where (4.10) follows from (4.6). So, it suffices to show

$$\limsup_{\epsilon \downarrow h} \sum_{k=1}^{\infty} P\left(D_k - \mu_k \leq -(\epsilon - h)s_k - a_k\right) \leq \alpha.$$

To apply part (ii) of Fatou's lemma, we first show that right-hand side of (4.10) is bounded above. To this end, consider $\gamma_0 > 0$ in (4.8),

$$\begin{aligned} & \sum_{k=1}^{\infty} P\left(D_k - \mu_k \leq -(\epsilon - h)s_k - a_k\right) \\ \leq & \sum_{k=1}^{\infty} P\left(D_k - \mu_k \leq -a_k\right) \\ \leq & \sum_{k=1}^{\infty} \int_{\hat{x}_k} P\left(D_k - \mu_k \leq -a_k \mid \hat{x}_k\right) dP_{\hat{x}_k} \qquad (4.11) \\ \leq & \sum_{k=1}^{\infty} \int_{\hat{x}_k} E\left[e^{-\gamma_0\left(\frac{D_k - \mu_k}{\sigma_k/\sqrt{n_k}}\right)} \middle| \hat{x}_k \right] e^{-\frac{\gamma_0}{M}\left(a_k\sqrt{n_k}\right)} dP_{\hat{x}_k} \qquad (4.12) \\ \leq & \sup_k E\left[e^{-\gamma_0\left(\frac{D_k - \mu_k}{\sigma_k/\sqrt{n_k}}\right)} \right] \sum_{k=1}^{\infty} k^{-\left(\frac{\gamma_0\sqrt{2p}}{M(\epsilon - h)}\right)} \qquad (4.13) \end{aligned}$$

where (4.12) follows from an application of Chernoff bounds e.g., [52] to the conditional probability in (4.11). Note that for $\hat{x}_k$ with $\sigma_k^2 = 0$, the probability

in (4.11) is 0. Taking $p > \frac{M^2(\epsilon-h)^2}{2\gamma_0}$, we have the right-hand side of (4.13) bounded. Taking limits we obtain,

$$\begin{aligned}
& \limsup_{\epsilon \downarrow h} \sum_{k=1}^{\infty} P\left(D_k - \mu_k \leq -(\epsilon - h)s_k - a_k\right) \\
\leq & \sum_{k=1}^{\infty} \limsup_{\epsilon \downarrow h} P\left(D_k - \mu_k \leq -(\epsilon - h)s_k - a_k\right) \\
\leq & \sum_{k=1}^{\infty} \limsup_{\epsilon \downarrow h} \int_{\hat{x}_k} P\left(\frac{D_k - \mu_k}{s_k/\sqrt{n_k}} \leq -(\epsilon - h)\sqrt{n_k} \middle| \hat{x}_k\right) dP_{\hat{x}_k} \\
\leq & \sum_{k=1}^{\infty} \int_{\hat{x}_k} \limsup_{\epsilon \downarrow h} P\left(\frac{D_k - \mu_k}{\sigma_k/\sqrt{n_k}} \leq -(c_p + 2pa_k^{-2}\ln^2 k)^{1/2}\left(\frac{s_k}{\sigma_k}\right) \middle| \hat{x}_k\right) dP_{\hat{x}_k} \\
\leq & \alpha,
\end{aligned}$$

where the first and the third inequalities follow from an application of Fatou's lemma. With $\hat{x}_k$ fixed, $\frac{D_k-\mu_k}{\sigma_k/\sqrt{n_k}}$ converges to a standard normal by the CLT and $\limsup_{\epsilon\downarrow h}(s_k/\sigma_k) \geq 1$, by Proposition 2.1. Then, the last inequality follows from application of Lemma 4.2 and the definition of c_p. □

Theorem 4.3 shows that for values of ϵ close enough to h, or, when the sample sizes n_k are large enough, we have the optimality gap of the solution when we stop within $[0,\ \epsilon s_T + a_T + \epsilon']$ with at least the desired probability of $1 - \alpha$. We now turn our attention to finite stopping and show that the sequential procedure stops with probability one. We state this formally in the proposition below.

Proposition 4.4. *Assume (A1)-(A3) and that $\tilde{\xi}^1, \tilde{\xi}^2, \ldots$ are i.i.d. as $\tilde{\xi}$, and assume (4.8) holds. Let $\epsilon' > 0$. Then, for the sequential sampling procedure*

where the sample size is increased according to (4.5), and the procedure stops at iteration T according to (4.3), we have $P(T < \infty) = 1$.

Proof. $P(T = \infty) \leq \limsup_{k\to\infty} P(G_k > hs_k + \epsilon') = 0$, where the last equality follows from the fact that $\epsilon' > 0$ and $\lim_{k\to\infty} G_k = 0$, and $\limsup_{k\to\infty} s_k \geq 0$, w.p.1. □

When X^* is a singleton, $(G_k, s_k) \to (0, 0)$ as $k \to \infty$, w.p.1. If we set $\epsilon' = 0$, we need to know the rate at which G_k and s_k tend to 0 as $k \to \infty$. With $\epsilon' > 0$, we are guaranteed of finite stopping with probability one for any value of $h > 0$. Kleywegt et al. [39] show for a class of stochastic discrete optimization problems with a unique optimum that $x_n^* = x^*$, w.p.1 for n large enough. In this case, there exists a K such that for $k \geq K$, both G_k and s_k are zero, w.p.1. Then, we can set $\epsilon' = 0$ and have a finite stopping time. However, this is not true in general. To see when things could go wrong with $\epsilon' = 0$, consider the following example.

Example 4.1. *Consider the following problem,* $\{\min E[\tilde{\xi}x - 0.5x] : 0 \leq x \leq 1\}$*, where* $\tilde{\xi}$ *has an exponential distribution with mean 1. Note that (A1)-(A3) are satisfied. The optimal solution to this problem is* $x^* = 0$ *with optimal value* $z^* = 0$*. Suppose we run the sequential procedure with parameters* $\epsilon' = 0$ *and* $h < 0.5$*. Suppose the candidate solutions are given as* $\hat{x}_k = 1/k$*, which satisfy the assumption* $\hat{x}_k \to x^*$*, w.p.1, required by the sequential procedure. As* $k \to \infty$*,* $G_k/s_k \to \mu_k/\sigma_k$*, w.p.1, where* $\mu_k/\sigma_k = 0.5$ *for all* k*. This implies, by convergence in probability that for any* $\varepsilon > 0$*,* $P(|G_k/s_k - 0.5| < \varepsilon) \to 1$*.*

Therefore, there is be a positive probability that the procedure does not stop, i.e. $P(T = \infty) > 0$*, when* $h < 0.5$*.*

4.3.2 Weaker Moment Conditions

In this section, we prove a version of Theorem 4.3 that assumes finite absolute moments up to r, instead of existence of an MGF. We relax the MGF assumption given in (4.8) to

$$E \sup_{x \in X} |f(x, \tilde{\xi})|^r < \infty, \tag{4.14}$$

for some integer $r \geq 2$. When $r = 2$, (4.14) is equivalent to assumption (A2). Note that (4.14) implies $\sup_{x \in X, y \in X^*} E|f(x, \tilde{\xi}) - f(y, \tilde{\xi})|^r < \infty$. Under this assumption, at each iteration k, we select the sample sizes according to

$$n_k \geq \left(\frac{1}{\epsilon - h} \right)^2 (c_p + 2p\, g(k)), \tag{4.15}$$

where $c_p = \max\{2 \ln \left(\sum_{k=1}^{\infty} k^{-p\, g(k)} / \sqrt{2\pi}\alpha \right), 1\}$. The growth in the sample size is of order $O(g(k))$, where $g(k) = k^{2/r} a_k^{-2} (\ln k)^{4/r}$. For example, when we use $a_k = 1/\sqrt{k}$, for $r = 2$, we have $g(k) = k^2 \ln^2 k$. Similarly, for $r = 4$, we have $g(k) = k^{1.5} \ln^2 k$. In other words, the less restrictive the assumption we make on the existence of moments, the higher the rate of growth in the sample sizes need to be.

We now formally state the validity and finite stopping of our procedure under the finite r^{th} moment assumption given in (4.14). We start with a lemma that establishes a bound on the absolute central moments of a sample mean.

Lemma 4.5. *Let $X^1, X^2, \ldots, X^n$ be a sequence of i.i.d. random variables with mean μ and $\bar{X}_n = \frac{1}{n}\sum_{i=1}^{n} X^i$. If $E|X^1 - \mu|^r < \infty$ for some integer r, then,*

$$E\left|\bar{X}_n - \mu\right|^r \leq E|X^1 - \mu|^r \left(\frac{r}{n}\right)^{r/2}.$$

Proof. The proof is essentially the same as that of Lemma 4.12 in [44, p. 86]. □

Theorem 4.6. *Assume (A1)-(A3) and that $\tilde{\xi}^1, \tilde{\xi}^2, \ldots$ are i.i.d. as $\tilde{\xi}$, and assume (4.14) holds. Let $p > 0$ and $0 < \alpha < 1$. Then, for the sequential sampling procedure where the sample size is increased according to (4.15), and the procedure stops at iteration T according to (4.3),*

$$P(T < \infty) = 1 \quad \textit{and} \quad \liminf_{\epsilon \downarrow h} P\left(\mu_T \leq \epsilon s_T + a_T + \epsilon'\right) \geq 1 - \alpha.$$

Proof. The proof of the finite stopping result is identical to that of Proposition 4.4. To prove asymptotic validity, we start as the proof of Theorem 4.3 and proceed until (4.11) the same way. Then, instead of using a Chernoff bound, which is Markov's inequality applied to the exponent of a random variable, we

use Markov's inequality with rth moment under the assumption of (4.14),

$$\begin{aligned}
& \sum_{k=1}^{\infty} \int_{\hat{x}_k} P\left(D_k - \mu_k \leq -a_k \mid \hat{x}_k\right) dP_{\hat{x}_k} \\
\leq & \sum_{k=1}^{\infty} \int_{\hat{x}_k} P\left(|D_k - \mu_k| \geq a_k \mid \hat{x}_k\right) dP_{\hat{x}_k} \\
\leq & \sum_{k=1}^{\infty} \int_{\hat{x}_k} E\left[|D_k - \mu_k|^r \mid \hat{x}_k\right] \; a_k^{-r} \; dP_{\hat{x}_k} \\
\leq & \sup_k E\left[|f(\hat{x}_k, \tilde{\xi}) - f(x^*_{\min}, \tilde{\xi}) - \mu_k|^r\right] \; r^{r/2} \sum_{k=1}^{\infty} \frac{1}{n_k^{r/2} a_k^r}, \qquad (4.16)
\end{aligned}$$

where (4.16) follows from Lemma 4.5. From the definition of n_k given in (4.15), the right-hand side of (4.16) is bounded. The rest of the proof is analogous to that of Theorem 4.3. □

Theorem 4.6 is different from Theorem 4.3 in that the finite MGF assumption of (4.8) is replaced by the finite r^{th} absolute moment assumption of (4.14), for $r \geq 2$. Under this assumption, the sample sizes are chosen according to (4.15) instead of (4.5). A closer look at the sample size formulas shows that the *lower bound* on the growth of sample size is $O(k \ln^2 k)$ for finite second moments, whereas it is $O(\ln^2 k)$ when MGF exists. In the previous chapter we have shown that, when $\hat{x}$ is fixed, it is possible design sequential procedures for assessing solution quality by increasing the sample size one by one, which corresponds to a growth of order $O(k)$ through the fully sequential procedure, under (A2), i.e. finite second moment assumption. When we allow $\hat{x}$ to change, we need the sample sizes to grow *at least* of order $O(k \ln^2 k)$, under the same assumption which is slightly larger than $O(k)$.

So far, we have proved several desired theoretical properties of our sequential procedure. In the next section, we discuss issues that arise when implementing the procedure. Then, we test its performance on two two-stage stochastic linear programs with recourse. These test problems satisfy (A1)-(A3) and their random vector $\tilde{\xi}$ has a discrete distribution with independent components each with bounded support. Therefore, the MGF assumption is automatically satisfied for all γ_0. Thus, in the next section, we discuss the implementation of our procedure under this assumption. The analysis is similar under the r^{th} absolute moment assumption.

4.4 Implementation

We start with a step by step summary of the sequential sampling procedure. We then discuss how to choose the parameter p, which appears in the definition of the sample size n_k in (4.5), to minimize the number of observations used for a given iteration number.

4.4.1 Algorithm

Below we state the sequential sampling procedure that uses the single replication procedure (SRP) of Section 2.2 to assess the quality of the sequence of candidate solutions.

Sequential Sampling Procedure:

Input: Desired values for $\epsilon, h, \epsilon' > 0$, and $0 < \alpha < 1$. Desired inflation factor a_k such that $a_k \downarrow 0$ as $k \to \infty$; a method that generates candidate solutions

$\{\hat{x}_k\}$ with limit points in X^*.

Output: A candidate solution, $\hat{x}_T$, and a $(1-\alpha)$-level confidence interval on the optimality gap of the candidate solution, $\mu_{\hat{x}_T}$.

0. (Initialization) Set $k = 1$, select p and calculate n_k as given in (4.5). Sample i.i.d. observations $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^{n_k}$ from the distribution of $\tilde{\xi}$,

1. Solve (SP_{n_k}) using observations generated so far to obtain $x^*_{n_k}$,

2. Calculate $G_k = \frac{1}{n_k}\sum_{i=1}^{n_k}\left(f(\hat{x}_k, \tilde{\xi}^i) - f(x^*_{n_k}, \tilde{\xi}^i)\right)$, and
$s_k^2 = \frac{1}{n_k - 1}\sum_{i=1}^{n_k}\left[(f(\hat{x}_k, \tilde{\xi}^i) - f(x^*_{n_k}, \tilde{\xi}^i)) - (\bar{f}_{n_k}(\hat{x}_k) - \bar{f}_{n_k}(x^*_{n_k}))\right]^2$.

3. If $\{G_k \leq hs_k + \epsilon'\}$, then set $T = k$, and goto 4.

Else, calculate n_{k+1}, sample $n_{k+1} - n_k$ i.i.d. observations $\tilde{\xi}^{n_k+1}, \tilde{\xi}^{n_k+2}, \ldots, \tilde{\xi}^{n_{k+1}}$ from the distribution of $\tilde{\xi}$. Set $k = k + 1$ and goto 1.

4. Output candidate solution $\hat{x}_T$ and a one-sided CI on $\mu_{\hat{x}_T}$,

$$[0,\ \epsilon s_T + a_T + \epsilon'] \,. \tag{4.17}$$

The implementation of the sequential procedure with A2RP involves small changes. We select n_k *even* and divide the observations into two random partitions and calculate G_k^i and $s_k^{2\,i}$ for each sample $i = 1, 2$. We then use the pooled gap and variance estimates as given in (2.10) for the stopping criterion in step 3. It is easy to verify that the theoretical properties presented in the previous section remain valid for A2RP. In our computational tests, we also use

ε-optimal versions of these methods in which we solve the sampling problem(s) in step 1 suboptimally.

Above, the method that generates candidate solutions is an input to the sequential procedure. This method can be anything as long as the sequence of candidate solutions have limit points in the set of optimal solutions, X^*. In our computational results, we generate the candidate solutions $\{\hat{x}_k\}$ by solving a separate sampling problem (SP_{m_k}) with increasing sample sizes m_k at iteration k. Briefly, we state it below.

Generating candidate solutions:

i. Set $m_k = m_1$. Sample i.i.d. observations (independent of those in the above sequential procedure) $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^{m_k}$ from the distribution of $\tilde{\xi}$,

ii. Solve (SP_{m_k}) using observations generated so far to obtain $x^*_{m_k}$,

iii. Set $\hat{x}_k = x^*_{m_k}$. Calculate m_{k+1}, sample $m_{k+1} - m_k$ i.i.d. observations $\tilde{\xi}^{m_k+1}, \tilde{\xi}^{m_k+2}, \ldots, \tilde{\xi}^{m_{k+1}}$ from the distribution of $\tilde{\xi}$. Set $k = k+1$ and goto *ii.*

Note that in step i above, we generate observations that are independent from the ones used in steps 0 and 3 of the sequential procedure. We are now ready to discuss more specific implementation issues, such as how to choose sample sizes by adjusting the value of the parameter p.

4.4.2 How to choose p

In this section, we discuss how to choose p to minimize the computational effort exerted by the by the sequential procedure. In our computational

results, we use $a_k = 1/\sqrt{k}$. This corresponds to taking the sample sizes as

$$n_k \geq \left(\frac{1}{\epsilon - h}\right)^2 \left(c_p + 2pk \ln^2 k\right), \tag{4.18}$$

where $c_p = \max\{2 \ln \left(\sum_{k=1}^{\infty} k^{-pk \ln k}/\sqrt{2\pi}\alpha\right), 1\}$. The parameter p that appears in the constant term, c_p, and the growth term, $2pk \ln^2 k$, allows us to adjust the number of samples we use at each iteration. Note that in Theorem 4.3, we require $p > (\epsilon - h)^2 M^2 / 2\gamma_0^2$. This may prevent us from optimizing the value of p since we do not know the lower bound on p, but if, e.g., the underlying random parameters have bounded support then the moment generating function assumption of (4.8) is satisfied for all γ. In this case, we can use any $p > 0$. Following a similar analysis as in [45], in this section we find the value of $p > 0$ that minimizes the computational effort, which can be approximated by the sum of sample sizes.

Suppose we wish to have a maximum of T iterations. The actual number of iterations of the procedure is unknown, as it is a random variable. However, by assuming a certain number of iterations, T, we can find the optimum p for this T and then run the procedure with this p. We are willing to accept a slightly suboptimal value of p, when the algorithm terminates with an actual number of iterations that deviates a bit from our guess. For a fixed number of iterations T, the sum of n_k's is proportional to

$$S(p) = T \max\left\{2 \ln\left(\frac{\sum_{k=1}^{\infty} k^{-pk \ln k}}{\sqrt{2\pi}\alpha}\right), 1\right\} + 2p \sum_{k=1}^{T} k \ln^2 k,$$

with the proportionality constant of $(\epsilon - h)^{-2}$. Our aim is to minimize $S(p)$, for $p > 0$. It is possible to show that $S(p)$ is a convex function.

Proposition 4.7. *$S(p)$ is a convex function on $p > 0$.*

Proof. It is sufficient to show that $\ln\left(\sum_{k=1}^{\infty} k^{-pk\ln k}\right)$ is a convex function on $p > 0$. Let $\Psi(p) = \sum_{k=1}^{\infty} k^{-pk\ln k}$. We need to show $\ln\Psi(\lambda p_1 + (1-\lambda)p_2) \leq \lambda \ln\Psi(p_1) + (1-\lambda)\ln\Psi(p_2)$ for all $p_1, p_2 > 0$ and $0 \leq \lambda \leq 1$. After some algebra, we see that this is equivalent to showing

$$\sum_{k=1}^{\infty}\left(k^{-p_1 k\ln k}\right)^{\lambda}\left(k^{-p_2 k\ln k}\right)^{1-\lambda} \leq \left[\sum_{k=1}^{\infty} k^{-p_1 k\ln k}\right]^{\lambda}\left[\sum_{k=1}^{\infty} k^{-p_2 k\ln k}\right]^{1-\lambda}.$$

This inequality follows from an infinite series version of Hölder's inequality [12, p.181]. □

Minimizing the convex univariate function $S(p)$ with respect to p is computationally straightforward. Table 4.1 shows the optimum value of p^* for different values of T, and the value of $S(p^*)$ when $\alpha = 0.10$ or 0.05. Note that larger sample sizes are needed for a higher confidence level. From (4.5), the sample size growth is bounded below by $O(\ln^2 k)$, which corresponds to $n_k \geq (\epsilon - h)^{-2}\left(c_p + 2p\ln^2 k\right)$, with $c_p = \max\{2\ln\left(\sum_{k=1}^{\infty} k^{-p\ln k}/\sqrt{2\pi}\alpha\right), 1\}$. Comparing this extreme case with the $O(k\ln^2 k)$ growth examined in this section, we note that both p^* and $S(p^*)$ decrease for a fixed value of T as the order of growth changes from $O(\ln^2 k)$ to $O(k\ln^2 k)$. For instance, $p^* = 1.55\times10^{-1}$ with $S(p^*) = 1{,}473$ ($\alpha = 0.05$) for T =100, and $p^* = 9.0\times10^{-2}$ with $S(p^*) = 19{,}720$ (again, $\alpha = 0.05$) for T =1,000, for $O(\ln^2 k)$ growth [45].

We note that it is possible to implement the sequential sampling procedure such that the value of p is changed during the algorithm. For instance, we

T	p^*	$S(p^*)$	
		$\alpha = 0.10$	$\alpha = 0.05$
10	2.7×10^{-2}	78	92
50	2.1×10^{-3}	553	622
100	8.0×10^{-4}	1,245	1,384
500	1.0×10^{-4}	7,852	8,542
1000	3.7×10^{-5}	17,092	18,483

Table 4.1: Choice of p that minimizes $S(p)$ for a given number of iterations, T.

can start with $p^1 = 2.1 \times 10^{-3}$ assuming $T = 50$, and when the algorithm goes beyond a certain iteration number, say, 80, we can switch to $p^2 = 8 \times 10^{-4}$ for $T = 100$. Note that we also need to adjust the value of c_p. This way, we can reduce the computational effort by reducing the number of times new samples are added. That said, in our computational results we fix the value of p, assuming an average number of iterations T and do not change it within the algorithm. Even when the procedure terminates at a different iteration than that of the assumed T, the differences in sample sizes are quite modest. For instance, taking $\epsilon - h = 0.5$ and $\alpha = 0.10$, and using $p^1 = 2.1 \times 10^{-3}$, we have $n_T \geq 40$, 52, and 75 samples when $T = 1$, 50 and 100, respectively. Similarly, we have $n_T \geq 45$, 50, and 58 when we instead use $p^2 = 8 \times 10^{-4}$.

4.5 Computational Results

We have applied the sequential sampling procedure described above to two two-stage stochastic linear programs from the literature, PGP2 and APL1P. These two problems were also studied in Chapter 2. Recall that

PGP2 is an electric power generation model with 3 stochastic parameters and 576 scenarios. APL1P, another power generation model, has 5 independent stochastic parameters and 1280 scenarios. Both of the problems satisfy (A1)-(A3) stated in Section 1.2 and the MGF assumption (4.8). For more details on the test problems, please refer to Section 2.4.2. We specifically use these as test problems since they pose challenges for our optimality gap estimates.

When implementing the procedure, we set $\epsilon' = 1 \times 10^{-7}$, which in addition to ensuring finite stopping, serves to deal with nonzero numerical tolerances. For instance, suppose we are using a solver with a tolerance of 1×10^{-8} and at an iteration k, we calculate $G_k = 1 \times 10^{-8}$ and $s_k = 1 \times 10^{-12}$, which we can essentially treat as 0. However, if we do not have ϵ' in (4.3), we would not stop for $h < 10^4$.

We take $a_k = 1/\sqrt{k}$, and therefore, use the sample size formula given in (4.18). We set $\alpha = 0.10$ and design the procedure for $T = 50$, setting $p = 2.1 \times 10^{-3}$ and $c_p = 9.7667$. Table 4.2 lists the values of h and ϵ used for the two test problems PGP2 and APL1P. With the given parameters, the sequential procedure uses $n_1 \geq 100$ for PGP2 and $n_1 \geq 200$ for APL1P. Even though it is possible to take sample sizes larger than these, in our tests, we used the minimum possible number of sample sizes at each iteration.

To generate the candidate solutions we use a separate stream of i.i.d. observations from the distribution of $\tilde{\xi}$, as described above. We set $m_1 = n_1$, that is, $m_1 = 100$ for PGP2 and $m_1 = 200$ for APL1P. Then, we set $m_{k+1} = m_k + 5$. In other words, at each iteration k, we add five observations and use

	PGP2	APL1P
h	0.086	0.054
ϵ	0.400	0.275
n_1	100	200

Table 4.2: Parameters and the corresponding initial sample sizes used in the tests. Other parameters are the same for both test problems: $\alpha = 0.10$, $\epsilon' = 1 \times 10^{-7}$, $p = 2.1 \times 10^{-3}$ and $c_p = 9.7667$.

the solution to this sampling problem, $x^*_{m_k}$ as $\hat{x}_k$. Both test problems have small numbers of scenarios; so, when the sample size exceeds the cardinality of the sample space, we continue sampling, albeit at a slower rate. After this point we set $m_{k+1} = m_k + 2$.

As before, for our computational results, we used the regularized decomposition algorithm [55]. An accelerated implementation of this algorithm, in C++, is due to Ruszczyński and Świetanowski [57]. We have modified this code to warm-start the algorithm when an additional scenario or a number of scenarios is added to the current problem allowing for faster solution times in sequential sampling. We tested four different methods to assess a candidate solution's quality within the sequential procedure, namely, SRP, A2RP and their ε-optimal versions. For the ε-optimal procedures, we set the suboptimality level to 1.75×10^{-3}, which was found to yield good coverage results in Chapter 2. Using each of the procedures for assessing solution quality, we repeat the sequential procedure 100 times and report empirical coverage probabilities, $\hat{p}$. This is an estimate of the probability that the CI produced at the end of the sequential procedure, $[0,\ \epsilon s_T + a_T + \epsilon']$, contains the optimality

Method	T	μ_T	$\epsilon s_T + a_T + \epsilon'$	$\hat{p}$
SRP	26.31 ± 8.20	0.78 ± 0.23	18.07 ± 4.28	0.75 ± 0.07
ε-Opt SRP	20.58 ± 5.19	0.78 ± 0.23	34.94 ± 12.14	0.98 ± 0.02
A2RP	72.26 ± 14.35	0.79 ± 0.23	23.18 ± 4.18	0.83 ± 0.06
ε-Opt A2RP	69.44 ± 12.80	0.79 ± 0.23	62.97 ± 18.50	0.98 ± 0.02

Table 4.3: Summary of results for PGP2. We report average values of T, the iteration the sequential procedure stopped; μ_T, the optimality gap of the candidate solution at the stopping iteration; $\epsilon s_T + a_T + \epsilon'$, the CI width on μ_T; and $\hat{p}$, an estimate of the coverage probability, $P\left(\mu_T \leq \epsilon s_T + a_T + \epsilon'\right)$. All of these values are reported along with their associated 90% CI widths.

Method	T	μ_T	$\epsilon s_T + a_T + \epsilon'$	$\hat{p}$
SRP	9.06 ± 2.92	15.09 ± 3.99	155.16 ± 20.30	0.97 ± 0.03
ε-Opt SRP	7.46 ± 2.28	16.29 ± 4.08	237.07 ± 61.59	0.97 ± 0.03
A2RP	18.99 ± 6.19	14.06 ± 4.25	197.68 ± 17.76	1 ± 0
ε-Opt A2RP	14.33 ± 4.04	14.62 ± 4.31	285.34 ± 45.14	1 ± 0

Table 4.4: Summary of results for APL1P.

gap of the candidate solution at the stopping iteration, μ_T. In other words, $\hat{p}$ estimates the probability in (4.4). To reduce the effect of sampling when comparing the results, we used the same stream of random numbers in each of the 100 repetitions for all of the methods. For instance, if SRP and ε-optimal SRP stop at the same iteration in one particular run, then they use the same observations and solve exactly the same sampling problems. The same is true for A2RP and ε-optimal A2RP. However, since we sometimes increase n_k to the nearest *even* number in A2RP methods, SRP and A2RP do not use exactly the same observations.

Tables 4.3 and 4.4 provide a summary of results for PGP2 and APL1P, respectively. The results indicate that the A2RP methods, on average, take

longer time to solve (T is larger) and have better coverage probabilities ($\hat{p}$ is larger). The ε-optimal versions stop slightly earlier than their counterparts that are solved to optimality. ε-optimal versions increase the coverage probabilities to desirable levels when solving PGP2 but they do not have much effect for APL1P.

The optimal value, z^*, for PGP2 is 447.324 and it is 24,642.32 for APL1P. The average optimality gap (μ_T) of the solutions obtained using the sequential procedure are well within 1% of the optimal for both problems. The CI width produced at the end of the procedure, $\epsilon s_T + a_T + \epsilon'$, is on average, larger than the average optimality gap. For APL1P, the CI widths are approximately within 1% of optimality. However, even though the coverage results are not always good for PGP2, the average CI widths are quite large. This is because the variance of the some of the frequently-obtained solutions are quite large. For example, x_1 given in Table 2.6 has a standard deviation of 82.69, see Table 2.2.

To examine this in more detail, we provide a histogram of μ_T and $\epsilon s_T + a_T + \epsilon'$ in Figures 4.1 and 4.2 for PGP2 and APL1P, respectively. The figures show the results for the sequential procedure that uses ε-optimal A2RP to assess solution quality. The CI width on the optimality gap of the candidate solution at the stopping iteration of the sequential procedure for PGP2, is usually much larger than the optimality gap of the candidate solution at the stopping iteration. The CI widths vary quite a lot for PGP2 and some are very large, around 450. Recall that $z^* = 447.324$ for PGP2. This is because

PGP2 has a large variance. One might try to control the sampling variance by adding an additional condition $\{s_k \leq b\}$ to the stopping criterion. However, in our computational results, we have seen that this sometimes results in very long runs, with $T \geq 2{,}000$. The CI widths for the APL1P, on the other hand, are not very large, even though they are usually somewhat larger than the optimality gaps. The CI widths in Figure 4.2 are at most 7% of the optimal value of APL1P.

4.6 Concluding Remarks

In this chapter, we have developed a sequential sampling procedure to solve stochastic programs. We assume a sequence of candidate solutions with limit points that solve (SP) are given and we assess their quality at each iteration. We increase the sample size until we reach a good solution, determined by a stopping criterion. We have proved desired theoretical properties under a finite moment generating function assumption and we have discussed the same properties under weaker moment conditions.

We tested our sequential sampling procedure using two two-stage stochastic linear programs with recourse, PGP2 and APL1P. We used four different methods to assess a candidate solution's quality that were previously developed in Chapter 2. These are SRP, A2RP, and their ε-optimal versions. Our preliminary computational results indicate that the sequential sampling procedure with ε-optimal A2RP yields good coverage results. However, when the underlying problem has a large variance, the resulting confidence interval

widths given in (4.17) can be quite large. For instance, we have seen this in PGP2. In contrast, the computational results for our other test problem, APL1P, yield solutions that have objective function values within 1% of the optimal value with very high probabilities.

An area of future research is to develop more efficient sequential sampling procedures while maintaining the desired asymptotic properties. We discuss this and other future research directions in more detail in the next chapter.

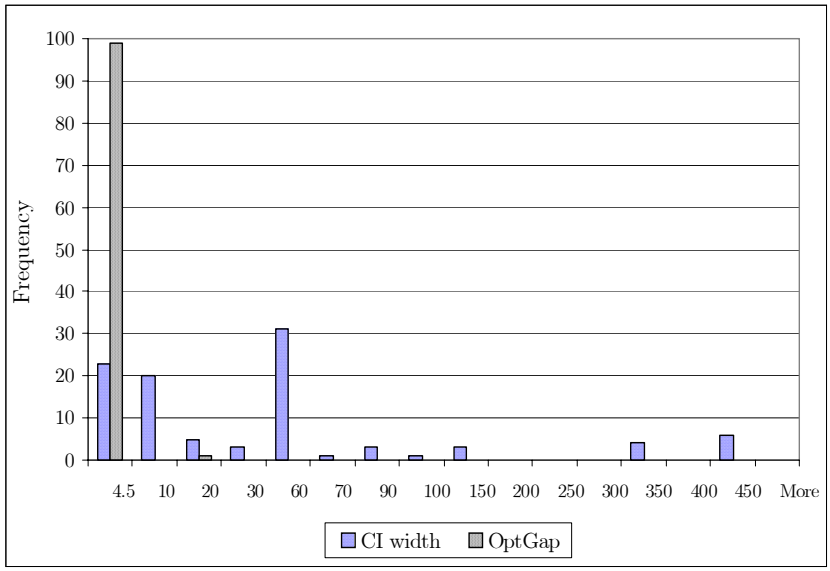

Figure 4.1: Histogram of μ_T (OptGap) and $\epsilon s_T + a_T + \epsilon'$ (CI width) out of 100 repetitions of the sequential procedure with ε-optimal A2RP for PGP2. (Note that the x-axis (cells of the histogram) does not have a uniform scale.)

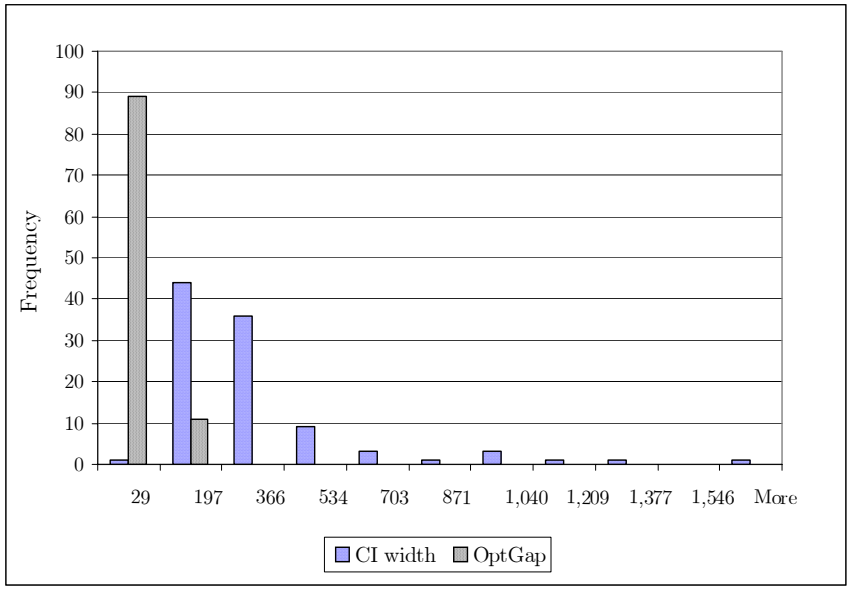

Figure 4.2: This figure is similar to Figure 4.1 except that it is for APL1P.

Chapter 5

Conclusions

In this dissertation, we have developed Monte Carlo sampling-based methods for stochastic programs, focusing on stochastic programs with recourse. Monte Carlo sampling-based methods provide an attractive approximation when the number of stochastic parameters in a stochastic program grows large. These methods replace the probabilistic statements that appear in the model (e.g., expectation) with their sampling estimators (e.g., sample mean). They are quite intuitive and while there is some research in this area, systematic guidelines for their implementation and theoretical results for their validity are still being developed. The research presented in this dissertation mainly addresses two issues that arise when using Monte Carlo sampling-based methods: assessing solution quality and sequential sampling procedures.

5.1 Summary of Contributions

Our specific contributions include the following.

- We have developed novel Monte Carlo sampling-based methods for assessing solution quality, which form a confidence interval on the optimality gap. Compared to an earlier method that requires solution of many

problems, our procedures require only solving one or two optimization problems.

- We have developed sequential sampling methods for assessing solution quality that control the sampling error. Analysis of sequential methods requires more care, and we have proved asymptotic validity of these procedures' confidence intervals similar to their fixed-sample counterparts.

- We have proposed a sequential sampling procedure to solve stochastic programs. Our method provides rules to increase the sample size, and a stopping criterion that determines when the current candidate solution has an objective function value close to the optimal value. We show that this procedure stops in a finite number of steps and asymptotically produces a high quality solution with a high probability.
- For all of our procedures, we present computational results that reveal insights as to how the procedures perform for small sample sizes.

We note that the results on assessing solution quality can be used within or after any method that provides an approximate solution to (SP). In our sequential procedure, for instance, we have used the single and two-replication procedures developed in Chapter 2. In the next section, we briefly discuss future research directions that branch out from the research presented in this dissertation.

5.2 Future Research Directions

There are several important extensions of the research presented in this dissertation. For instance, the sequential sampling procedures presented in Chapter 3 assume unique optimality. In the context of strict convexity in a nonlinear stochastic program, unique optimality may arise naturally but many linear problems have multiple optimum solutions. Therefore, extensions of the results presented in Chapter 3 that relax the unique optimality condition will make them more applicable. As before, this needs to be handled carefully as we are dealing with random sequences and subsequences. Below, we discuss three other important future research directions in more detail.

Adaptive Sequential Methods:

The sequential sampling procedure presented in Chapter 4 can be made adaptive, where the sampling method takes into account the information obtained about the problem so far. Carefully designed adaptive methods can be more efficient while maintaining the desired asymptotic properties. This merits further investigation.

Extension to Stochastic Integer Programs:

Many problems of practical interest can only be modeled using integer variables and it would be beneficial to extend the results of the dissertation to stochastic integer programs. Recall that in our results, we have assumed (A1), i.e., that $f(\cdot, \tilde{\xi})$ is continuous on X, w.p.1. This assumption eliminates consideration of two-stage stochastic integer programs when there are integrality

constraints in the second stage. We should note that when only the first stage decisions are discrete, our methods remain valid. We only need to change (A1) to $f(\cdot, \tilde{\xi})$ is continuous on $conv(X)$, w.p.1, where $conv(X)$ denotes the convex hull of X.

The asymptotic results on assessing solution quality and sequential sampling methods need to be approached more delicately when we lose the continuity assumption. An essential part of the proofs for assessing solution quality is the consistency of the variance estimator. All of the procedures developed can be proven valid if the consistency of variance estimator can be established. For instance, when there are integer constraints in the second stage of a two-stage stochastic program with recourse, the objective function $E[f(x, \tilde{\xi})]$ is lower-semi continuous on X. If it can be shown that the variance estimator is a consistent estimator of the true variance for lower-semi continuous functions, then these procedures can be readily applied to two-stage stochastic programs with integer recourse.

For small-sample behavior, we have observed that discreteness poses a practical challenge in assessing solution quality. It would be interesting to examine this effect in more detail for stochastic integer programs and try to develop methods to prevent undercoverage with small sample sizes.

Extension to Multi-Stage Models:

In our computational results, we have used two-stage stochastic linear programs with recourse. A future research topic of interest is to develop adap-

tive sequential sampling methods for multi-stage stochastic programs with recourse. In multi-stage models, solutions are represented as a *policy*, and the uncertainty is modeled as a stochastic process, which is either defined or approximated by a *scenario tree*. In this case, increasing the sample size corresponds to adding new branches to the scenario tree.

A sequential procedure for multi-stage models starts with a small scenario tree. The resulting approximating problem is solved, and new branches are sequentially added to the scenario tree until a desired precision is reached. The questions to be answered include: how to choose a starting tree; to which node to add new branches; how many new branches to add; how to assess a policy's quality and developing valid stopping rules.

On the computational side, multi-stage models are quite challenging to solve and their special structure can be exploited to gain efficiencies using parallel computing.

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